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PB-260 729

Development of a Mathematical Water Quality Model for Grays Harbor and the Chehalis River, Washington

Battelle Pacific Northwest Labs, Richland, Wash

Prepared for

Environmental Protection Agency, Washington, D C

Oct 74

PB 260 729

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SPRINGFIELD, VA. 22161

BIBLIOGRAPHIC DATA SHEET	1. Report No.	2.	3. Recipient's Accession No. PB-260 729
4. Title and Subtitle Development of a Mathematical Water Quality Model for Grays Harbor and the Chehalis River, Washington.			5. Report Date October 1974 6.
7. Author(s)			8. Performing Organization Rept. No.
9. Performing Organization Name and Address Battelle Pacific Northwest Laboratories Richland, Washington			10. Project/Task/Work Unit No. 11. Contract/Grant No.
12. Sponsoring Organization Name and Address			13. Type of Report & Period Covered 14.

15. Supplementary Notes

(PC A04/MF A01)

16. Abstracts

The objective of this study was to develop and apply a water quality model of the Grays Harbor Estuary and the Chehelis River. To accomplish this objective, the Battelle-Northwest water quality models EXPLORE-I (for tidally influenced systems) and PIONEER-I (for nontidal systems) were modified and calibrated to fit these specific situations. In this report, combined models simulate concentrations of water quality parameters.

17. Key Words and Document Analysis. 17a. Descriptors

*Water quality
*Mathematical models
*Grays Harbor Estuary
*Chehalis River
Simulation
Nitrogen
Salinity
Phosphorus
Ammonia
Biochemical oxygen demand
Chlorophylls
Oxygen
Dissolved gases
Coliform bacteria
Sulfites
Washington(State)

17b. Identifiers/Open-Ended Terms

*Model studies
Porter(Washington)

17c. COSATI Field Group 13B

18. Availability Statement	19. Security Class (This Report)	21. No. of Pages
National Technical Information Service Springfield, VA 22161	UNCLASSIFIED	67
	20. Security Class (This Page) UNCLASSIFIED	22. Price PC$4.50/ MF$3.00

FORM NTIS-35 (REV. 10-73) ENDORSED BY ANSI AND UNESCO. THIS FORM MAY BE REPRODUCED USCOMM-DC 8265-P74

DEVELOPMENT OF A MATHEMATICAL WATER QUALITY MODEL FOR GRAYS HARBOR AND THE CHEHALIS RIVER, WASHINGTON

DOCUMENTATION REPORT

211B01360

to

ENVIRONMENTAL PROTECTION AGENCY
Contract No. 68-01-1807

October 1974

PACIFIC NORTHWEST LABORATORIES
a division of
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SECTION I

SUMMARY AND CONCLUSIONS

This report documents the application of a mathematical hydrodynamic and water quality model to Grays Harbor and the Chehalis River, Washington. The EXPLORE-I code was applied to the tidally influenced portions of Grays Harbor and the PIONEER-I code, to the Chehalis River. Modifications were made to the EXPLORE-I code for this project, including: conversion to IBM computer, addition of "tide flat channels," options to specify quality of incoming seawater, options to use only a subset of model parameters, and conversion to metric units. The model was successfully calibrated and verified for dissolved oxygen in 1970, 1971 and 1972. Waste discharge and water quality data were obtained from extensive surveys supervised by the Washington State Department of Ecology. It was found that the quality of incoming seawater and benthic oxygen demand were extremely important variables affecting water quality in the Harbor and lower Chehalis River.

Lack of data precluded calibration and verification of PIONEER-I, although the model was set up and applied to the Chehalis River.

This report was submitted in fulfillment of Project #211B01360, Contract #68-01-1807 under the sponscrship of the U.S. Environmental Protection Agency.

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SECTION II

DEVELOPMENT OF A MATHEMATICAL WATER QUALITY MODEL FOR GRAYS HARBOR AND THE CHEHALIS RIVER, WASHINGTON

INTRODUCTION

The objective of this study was to develop and apply a water quality model of the Grays Harbor Estuary and the Chehalis River. To accomplish this objective, the Battelle-Northwest water quality models EXPLORE-I (for tidally influenced systems) and PIONEER-I (for nontidal systems) were modified and calibrated to fit these specific situations. PIONEER-I and EXPLORE-I have previously been applied to other river basin systems and are modified versions of the DOSAG and the STORM WATER MANAGEMENT (SWMM) models.

In this study the modified EXPLORE-I was applied to the tidally influenced portions of Grays Harbor Estuary, the Hoquiam and Wishkah Rivers, and the Chehalis River to Porter, Washington. PIONEER-I was used to simulate water quality conditions in the Chehalis River between Montesano and Chehalis. The two models overlap between Porter and Montesano since the closest upstream boundary condition for EXPLORE-I is the gauging station at Porter.

The combined models simulate concentrations of the following water quality parameters:

- Total nitrogen
- Salinity (chloride)
- Phosphorus (first or second order reaction)
- Coliform bacteria (first order reaction)
- Ammonia (first or second order reaction)
- Nitrite (first or second order reaction)
- Nitrate (first or second order reaction)
- Biochemical oxygen demand (first order reaction)
- Chlorophyll *a* (coupled with the nutrients in the phosphorus and nitrogen cycles)
- Dissolved oxygen (including benthic demand, BOD, ammonia and nitrite oxidation, and algal photosynthesis and respiration as functions of chlorophyll *a* concentration, time of day, and euphotic depth)
- Sulphite waste liquor (Pearl Benson Index)
- Toxic compound

This report documents the model's development and application to Grays Harbor and the Chehalis River. The EXPLORE-I code was extensively modified to fit the terms of the contract and to simulate the tide flat portions of the estuary. The revised code was calibrated and verified for oxygen predictions in the north channel area of the harbor and the lower Chehalis River.

The PIONEER-I code was converted to metric units and applied to the Chehalis River. Although a lack of data made calibration and verification of the PIONEER-I code impossible, the model was set up and run using reasonable parameter values in order to demonstrate its functions.

Three additional documents describe other aspects of this research program. The "System Layout and Data Report" details the mathematical representation of the system and summarizes hydraulic and water quality data. The "Sensitivity Analysis Report" documents the results of the sensitivity analyses which were performed in evaluating the model. The "User's Manual" provides detailed instructions for using the models. Program listings and source card decks are provided separately.

SECTION III

DESCRIPTION OF EXPLORE-I AS APPLIED TO GRAYS HARBOR

The mathematical model EXPLORE-I was developed by Battelle-Northwest for the Environmental Protection Agency to serve as a management tool in the allocation of water resources in a river basin. EXPLORE-I is a synthesis of a number of water quality models which have shown reliability in the past. The original code has been extensively documented by Battelle-Northwest.[1]

The EXPLORE-I code contains two basic components which are operated sequentially, a hydrodynamic component and a mass transport and water quality component. The hydrodynamic component calculates water flow, velocities, and surface elevations. The water quality component transports mass according to the calculated flows and calculates changes in constituent concentrations according to specified chemical and biological reactions.

Prior to the application of the mathematical model the system under study must be set up in a network of nodes and channels. The system used for Grays Harbor is described in detail in the "System Layout and Data Report."

HYDRODYNAMIC MODULE

The hydraulic simulation module of the EXPLORE-I code uses the equations of motion and continuity in conjunction with specified boundary conditions to calculate channel flows and consequent volume changes in nodes. Boundary conditions in the Grays Harbor study were upstream river flows and the tidal stage--time history at the estuary mouth. Upstream river flows can be time varying or constant. Constant values were used in this study.

The Saint-Venant equations of motion and continuity for open channel flow consist of two simultaneous equations:

Momentum

$$\frac{\partial V}{\partial t} + V\frac{\partial V}{\partial x} + g\frac{\partial h}{\partial x} = g\ (S_o - S_f + D_\ell) \qquad (1)$$

Continuity

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = q \qquad (2)$$

where

$V = Q/A$ = average velocity of flow, positive in downstream direction

$A = A[x,h(x,t)]$ = cross-sectional area of flow

Q = discharge across a section

h = depth of flow

q = lateral inflow, negative if outflow

S_o, S_f = bottom slope of channel and resistance slope

$$\left(S_f = \frac{n^2 |v| v}{2.2R^{4/3}}\right)$$

R = hydraulic radius

n = Manning's coefficient

D_ℓ = dynamic contribution of lateral discharge

x,t = space and time coordinates, respectively

The dynamic contribution of lateral inflow or outflow is given by

$$D_\ell = 0, \text{ for bulk lateral outflow}$$

$$D_\ell = \frac{Vq}{2Ag}, \text{ for seepage outflow}$$

$$D_\ell = \frac{V-u_\ell}{Ag} q, \text{ for lateral inflow}$$

where

u_ℓ = x-component of the inflow-velocity vector

The Saint-Venant equations can also be written with discharge instead of velocity as the primary kinetic variable. For flow through a rectangular cross section with negligible bottom slope and dynamic effect (of lateral inflow) these equations reduce to

Momentum

$$\frac{\partial V}{\partial t} + V\frac{\partial V}{\partial x} = -g\frac{\partial h}{\partial x} + gS_o - gS_f + gS_w \qquad (3)$$

Continuity

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial X} = 0 \qquad (4)$$

where

V = vertically averaged channel velocity

h = water depth

Q = volumetric flow rate

A = channel cross-sectional area (A-bh)

b = channel width

h = channel depth

S_w = wind stress term

The wind stress term S_w has been added to the traditional formulation to account for wind effects. In certain cases wind induced currents can be significant to the analysis of the flow patterns.

Most versions of the hydraulic model are formulated in terms of head (potential) instead of water depth, which has created some confusion about the correctness and completeness of the momentum and continuity equations. In previous versions of the hydraulic model the following substitutions were generally made (see Figure 1):

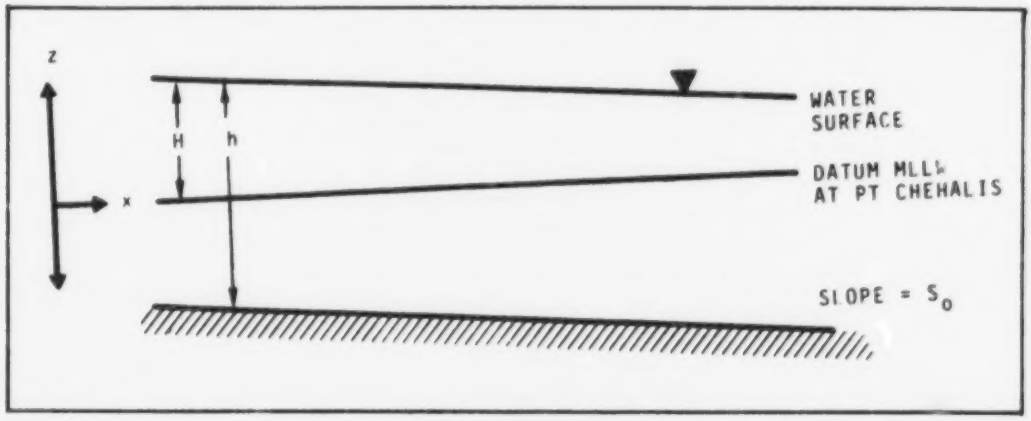


FIGURE 1. Diagram of Reference Plane Head (H) and Depth (h)

$$\frac{\partial h}{\partial t} = \frac{\partial H}{\partial t} \tag{5}$$

$$\frac{\partial H}{\partial X} = - \frac{\partial h}{\partial x} + S_o \tag{6}$$

$$S_o = - \frac{\partial z}{\partial x} \tag{7}$$

The bottom slope contribution S_o is generally small in estuarine applications. However, in river systems where changes in elevation provide the driving motion, these contributions can be significant.

A system is geometrically represented by a computational grid network. Using a simple routing concept, the flow in the system is prescribed along paths designated by channels connected by junctions. Each junction is characterized by its 1) surface area 2) water surface elevation, 3) bottom elevation, and 4) the actual (X,Y) coordinates. Surface areas are computed from the polygons formed by the perpendicular bisectors of channels in the network. Flow between these junctions occurs through rectangular channels connecting the junctions. The characteristics of each channel are described by length, width, Manning coefficient, and average bottom elevation at the mid-point. Figure 2 illustrates the channel-junction configuration.

In the numerical solution scheme, the Saint-Venant equations are not solved simultaneously for all points in the water system. Instead, the equation of motion, Equation 8, is solved for each of the channels in the system on the basis of present values of the junction heads.

Momentum

$$\frac{\partial V}{\partial t} = -V\frac{\partial V}{\partial x} - g\frac{\partial H}{\partial X} - gS_f + gS_w \tag{8}$$

where

V = velocity

H = water surface elevation measured from the datum plane

S_w = wind stress = $\frac{K}{h} \cdot \frac{\rho_a}{g\rho_w} U^2 \cos \psi$

K = dimensionless coefficient with a value of 0.0026

h = depth of flow

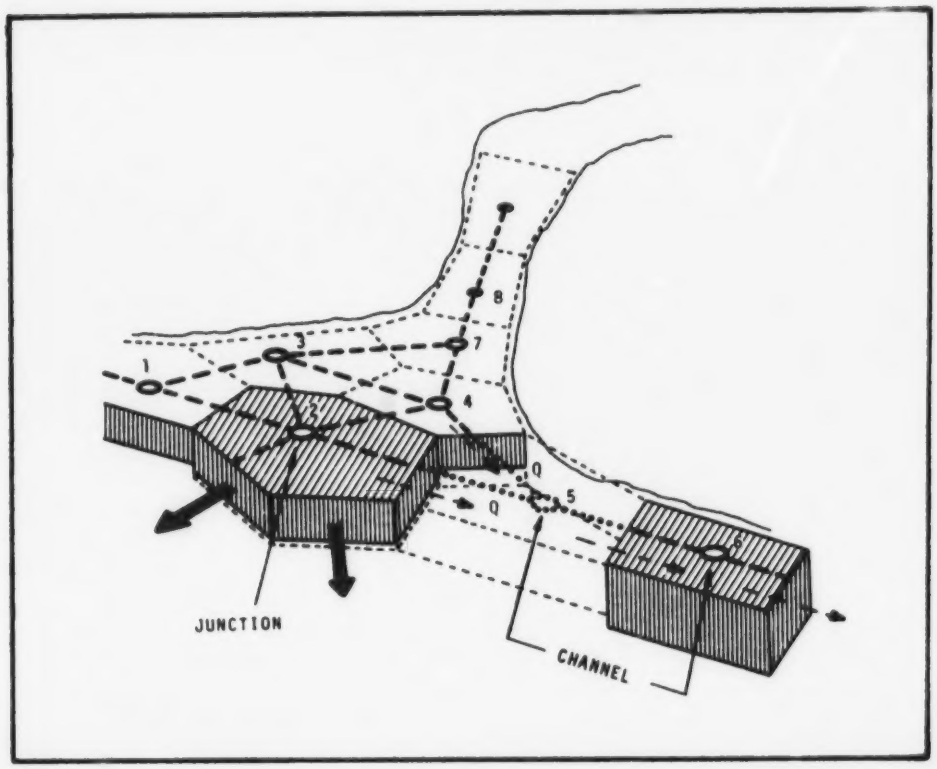


FIGURE 2. Channel-Junction Definition for Computational Mesh

ρ_a, ρ_w = air and water densities

U = wind velocity

ψ - angle between the wind direction and the axis of the channel

The velocity and flow in each of the channels is thus determined. The equation of continuity, Equation 9, is solved for each of the junctions on the basis of predicted flows in each of the channels.

Continuity

$$A_{sj} \frac{\partial H_j}{\partial t} = \sum_{i=1}^{k} Q_i + Q_j^{im} - Q_j^{ex} - Q_j^{ev} \qquad (9)$$

where

A_{sj} = surface area associated with the junction j

Q_i = flow of a connecting channel

$Q_j^{im}, Q_j^{ex}, Q_j^{ev}$ = water import, export and evaporation rates at the junction

k = number of channels connected to the j^{th} junction

The numerical integration technique employed in the hydraulic model uses a space- and time-staggered scheme based on a simple Runge-Kutta approximation. The finite-difference equation for the momentum equation may be expressed for the i^{th} channel as:

$$\frac{\Delta V_i}{\Delta t} = - V_i \frac{\Delta V_i}{\Delta x_i} - g\frac{\Delta h}{L_i} + gS_o - gK_j|V_i|V_i + gS_w \qquad (10)$$

where

V_i = channel velocity

Δt = time step

$\frac{\Delta V_i}{\Delta x_i}$ = velocity gradient

K_i = frictional resistance coefficient for channel i

g = acceleration of gravity

L_i = channel length

h = average channel depth

$\Delta h = h_j - h_{j+1}$

The velocity gradient term is computed from the continuity equation:

$$- V_i \frac{\Delta V_i}{\Delta x_i} = V_i \left[\frac{b_i}{A_i} \frac{\Delta h_i}{\Delta t} + \frac{V_i}{A_i} \frac{\Delta A_i}{L_i} \right] \qquad (11)$$

with

b_i = channel width

A_i = channel cross-sectional area

In addition, the relationships given below

$$\frac{\Delta h_i}{\Delta t} = \frac{\Delta H_i}{\Delta t}, \quad - g\frac{\Delta h}{L_i} + gS_o = - g\frac{\Delta H}{L_i} \tag{12}$$

and

$$\Delta A_i = b_i \Delta h_i \tag{13}$$

are used in intermediate computations of the key variables: V, h, Q, H, A. Since heads (potentials) are designated and computed at junctions the terms $\Delta H_i/\Delta t$ and $\Delta A_i/L_i$ are computed as the average of changes at the junctions at both ends of the channel.

The numerical solution technique proceeds as follows:

Initialization

1. Set initial and boundary flows and stages.

2. Set import and/or export flows.

3. Set water surface elevations and/or tidal conditions.

Leap-Frog Explicit Solution

1. Compute half-interval velocities, $V_i^{t+1/2}$ and quarter-interval channel flow, $Q_i^{t+1/4}$:

$$V_i^{t+1/2} = V_i^t + \frac{\Delta t}{2}\left[- V_i^t \frac{\Delta V_i^t}{\Delta x_i} - g\frac{\Delta h^t}{L_i} + gS_o - gK_i^t |V_i^t| V_i^t + gS_w \right]$$

$$Q_i^{t+1/4} = V_i^{t+1/2} A_i^t \tag{14}$$

2. Perform controlled junction calculations for flow at quarter-interval, Q_i^{t+4}, and head at half-interval, $H_j^{t+1/2}$. Head and/or flow may be specified functions of time or related via a rating curve.

3. Compute head at half-interval, $H_j^{t+1/2}$:

$$H_j^{t+1/2} = H_j^t + \frac{\Delta t}{2A_{sj}}\left[\sum_{i=1}^{k} Q_i^{t+1/4} + Q_j^{im} - Q_j^{ex} - Q_j^{ev}\right]$$

4. Compute half-interval flows, $Q_i^{t+1/2}$, and channel areas, $A_i^{t+1/2}$ and full-interval velocities, V_i^{t+1}:

$$A_i^{t+1/2} = A_i^t + b_i\left[\frac{\Delta H_j^{t+1/2} + \Delta H_{j+1}^{t+1/2}}{2}\right]$$

$$V_i^{t+1} = V_i^{t+1/2} + \Delta t\left[-V_i^{t+1/2}\frac{\Delta V_i^{t+1/2}}{\Delta x_i} - g\frac{\Delta h^{t+1/2}}{L_i} + gS_o - gK_i^{t+1/2}|V_i^{t+1/2}|V_i^{t+1/2}\right]$$

$$Q_i^{t+1/2} = 1/2\left[Q_i^{t+1/4} + V_i^{t+1}A_i^{t+1/2}\right]$$

5. Perform controlled junction calculations for flows and heads at full time step.

6. Compute full-interval heads, H_j^{t+1}; water depths, H^{t+1}; and channel areas, A_i^{t+1}:

$$H_j^{t+1} = H_j^{t+1/2} + \frac{\Delta t}{A_{sj}}\left[\sum_{i=1}^{k} Q_i^{t+1/2} + Q_j^{im} - Q_j^{ex} - Q_j^{ev}\right]$$

$$h_i^{t+1} = 1/2\left[\left(H_j^{t+1} - Z_j\right) + \left(H_{j+1}^{t+1} - Z_{j+1}\right)\right]$$

$$A_i^{t+1} = b_i\, h_i^{t+1}$$

7. Update system parameters and repeat steps 1 through 6 until hydraulic cycle is complete.

8. Average flows and velocities over hydraulic cycle.

This leap-frog scheme introduces a certain degree of accuracy and stability to the explicit numerical solution; however, there are inherent computational limitations. To maintain a stable and accurate solution the following criterion must be satisfied:

$$\Delta t_{max} \leq \frac{L_i}{\left[V_i \left(1 + \frac{gn^2 L_i}{2.2R^{4/3}}\right) + \sqrt{gR}\right]}$$

where

Δt_{max} = maximum time step for stable solution.

The expression in the brackets represents the celerity of a shallow water wave.

WATER QUALITY MODULE

The water quality module of EXPLORE-I consists of a mass transport submodel and a number of separate submodels for the various water quality parameters. All of these submodels are formulated from a mass balance on each constituent:

$$\begin{aligned}\text{Accumulation} = {} & \text{Advection} + \text{Diffusion} + \text{Import} - \text{Export} \\ & - \text{Settling} + \text{Scour} + \text{Reaeration} - \text{Decay} \\ & \pm \text{Chemical Transformation} \pm \text{Biological} \\ & \text{Transformations}\end{aligned} \quad (16)$$

The first five terms of this balance are the transport component while the remaining terms constitute the water quality submodels. Development of the EXPLORE-I multi-parameter water quality submodel involved formulating mathematical expressions for the kinetics of the individual mass transfer mechanisms.

In the mass transport/water quality submodels two basic assumptions are intrinsic:

- diffusion is negligible, and
- mass transfer is partitioned into simple transport and water quality kinetics.

The first of these was assumed for the estuary code because of the nebulous nature of hydrodynamic dispersion coefficients. Although literature on the subject is plentiful, no single equation or methodology is currently available which will accurately determine the mixing characteristics of

a general water body. In addition, investigations have shown that infinite-difference solutions to the advection-diffusion equation can introduce pseudo-dispersion effects which completely mask the actual solution. To avoid these difficulties and simplify data input specifications the diffusion term has been ignored.

The second assumption refers to the sequence of computations involved in the solution of the complete equations for species continuity.

For simplicity and convenience of computer implementation, the solution of the mass balance is partitioned into the sum of individual changes,

$$C^{k,n+1} + C^{k,n} + \Delta C^{k,n+1}_{transport} + \Delta C^{k,n+1}_{kinetics} \qquad (17)$$

where

$C^{k,n}, C^{k,n+1}$ = concentration of the k^{th} parameter at the old and new time planes

$\Delta C^{k,n+1}_{transport}$ = incremental change on the k^{th} parameter due to simple transport, i.e., advection, import and export

$\Delta C^{k,n+1}_{kinetics}$ = incremental change in the k^{th} parameter due to water quality kinetics, i.e., settling, scour, reaeration, decay, and chemical and biological transformations

The incremental change $\Delta^{k,n+1}_{transport}$ is obtained by finite-difference approximation from the solution of the partial differential equation for simple transport of each constituent. The incremental change $\Delta C^{k,n+1}_{kinetics}$ is determined from the simultaneous solution of the kinetic equations for all constituents by a 4th order Runge-Kutta scheme. Numerical experiments have shown that this form of approximation is adequate and greatly reduces the difficulty of the computational problem.

In choosing the models for each quality parameter, a number of guidelines were considered. Successful past use of a model was an important criterion. In addition, the simplest models which would provide acceptably accurate results were selected. Consideration was also given to the model's ease of calibration with existing water quality data.

The program consists of 12 integrated water quality submodels which predict the behavior of the water quality parameters. A diagram of the relationship between these submodels is shown in Figure 3; Table 1 is a list of the 12 water quality parameters.

TABLE 1. Water Quality Parameters Modeled in EXPLORE-I

1. Total nitrogen
2. Salinity
3. Soluble phosphorus
4. Coliform bacteria
5. Ammonia nitrogen
6. Nitrite nitrogen
7. Nitrate nitrogen
8. Biochemical Oxygen Demand
9. Phytoplankton
10. Dissolved oxygen
11. Sulphite waste liquor
12. Toxic compounds

Biochemical Oxygen Demand

The carbonaceous and nitrogenous components of BOD are combined so that the BOD equations become:

$$\frac{dL}{dt} = - (k_1 + k_3)L + P \qquad (18)$$

$$k_1 = k_1(20)\ \theta^{(T-20)} \qquad (19)$$

where

L = total BOD, mg/l

k_1 = deoxygenation coefficient: 0.1-0.8/day

k_3 = sedimentation coefficient: 0.0-3.5/day

P = scour coefficient: 0.0-0.8 mg/l-day

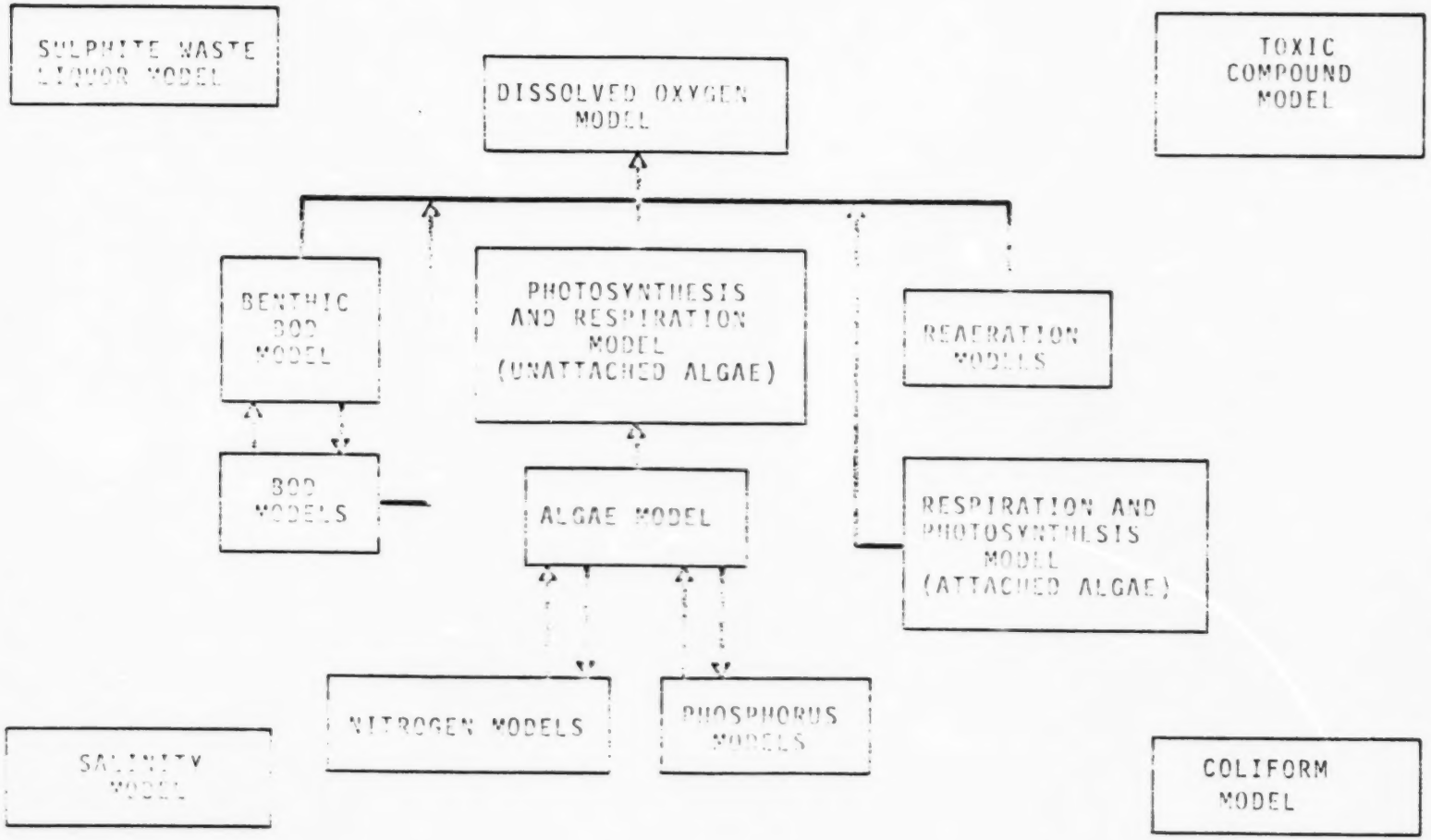


FIGURE 3. Integrated Models

$k_1(20)$ = deoxygenation coefficient at 20°C

θ = temperature coefficient: 1.05

T = temperature, °C

Sedimentation and scour terms were included in the BOD equation to allow the use of the model with different waste discharges and in varying hydraulic situations.

Benthic Oxygen Demand

The benthic oxygen demand is input as a rate of oxygen consumption. The value can be input by reach or node (see User's Manual).

$$\frac{dO_2}{dt} = \frac{1}{h} L_d \tag{20}$$

where

O_2 = oxygen concentration in overlying water, mg/l

h = water depth, meters

L_d = benthic oxygen demand, $g/m^2/day$

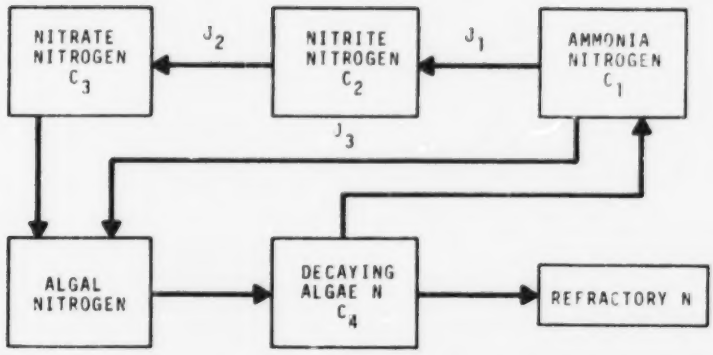
Nitrogen Model

Two nitrogen models have been included in the program. One incorporates the effects of algae while the second considers only ammonia-nitrate oxidation.

The algal nitrogen model (Figure 4A) assumes that each reaction can be described by a first order equation. The concentrations of the various nitrogen forms are given by C_i and the rates of reaction are given by J_i. The various nitrogen components were formulated as a first order model for two reasons. First, the relative simplicity of the first order equations with only one constant to be evaluated (along with the boundary conditions) is attractive. Detailed data for regression on a large number of constants will generally not be available. Second, the first order model has been shown to work satisfactorily, at least under certain conditions. The model is described by the equations:

$$\frac{dC_1}{dt} = - J_1C_1 + J_3C_4 - G_P P A_{NP} \left[\frac{C_1}{C_1+C_3}\right] \tag{21}$$

$$\frac{dC_2}{dt} = - J_2C_2 + J_1C_1 \tag{22}$$



A. ALGAL NITROGEN MODEL

B. FIRST ORDER NITROGEN MODEL

FIGURE 4. Nitrogen Models

$$\frac{dC_3}{dt} = J_2C_2 - G_P\ P\ A_{NP}\left[\frac{C_3}{C_1+C_3}\right] \qquad (23)$$

$$\frac{dC_4}{dt} = -\ J_3C_4 + D_PP\ A_{NP} \qquad (24)$$

where

C_1 = ammonia concentration, mg/l

C_2 = nitrite concentration, mg/l

C_3 = nitrate concentration, mg/l

C_4 = organic nigrogen concentration, mg/l

J_1, J_2, J_3 = rate constants: 0.1-0.5, 5.0-10.0, 0.1-0.4/day

P = phytoplankton concentration, mg-C/l

A_{NP} = ratio of nitrogen to carbon in phytoplankton: 0.17 mg-N/mg-C

G_P = growth rate of phytoplankton, day^{-1}

D_P = death rate of phytoplankton, day^{-1}

P, G_P, and D_P are formulated in the algae model

A simple first order ammonia-nitrate model (Figure 4B) has been included in the code for use when algal effects are not to be considered:

$$\frac{dC_1}{dt} = - J_2 C_1 \qquad (25)$$

$$\frac{dC_3}{dt} = + J_2 C_1 \qquad (26)$$

Phosphorus Model

Three phosphorus models are included in the quality model program. One includes the first order reactions of soluble phosphorus with algae and with the sediments (Figure 5A). The second is a first order reaction model between soluble and sediment phosphorus (Figure 5B). The third model is a second order decay model for soluble phosphorus (Figure 5C).

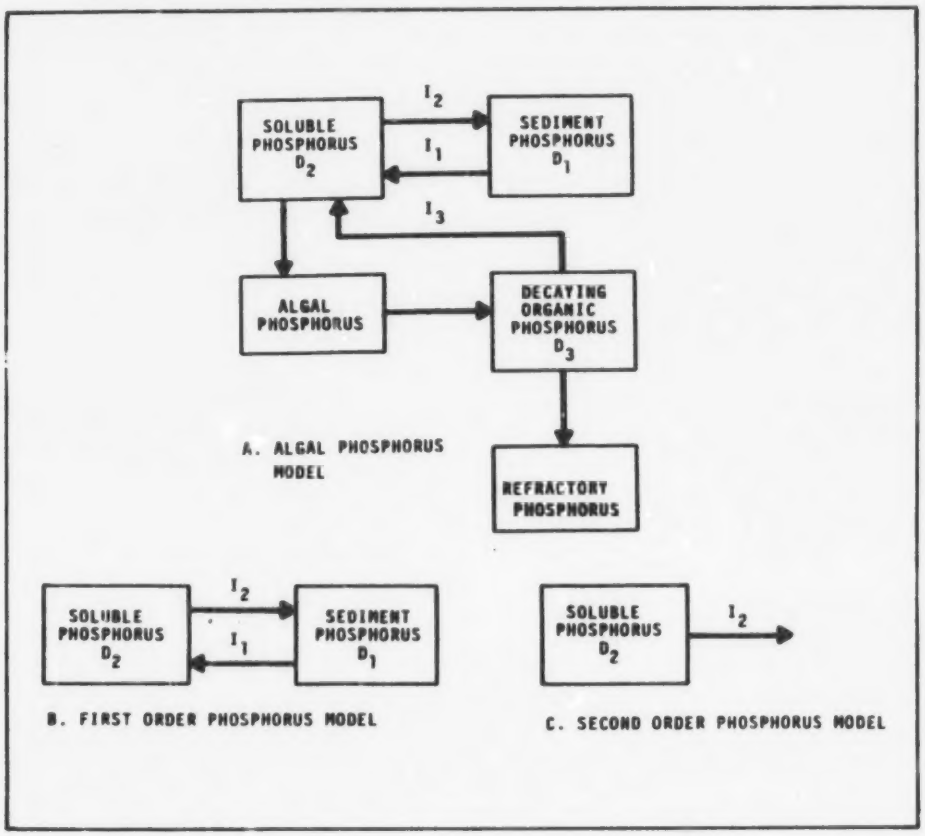


FIGURE 5. Phosphorus Models

The algal phosphorus model is similar to the nitrogen model and assumes that the reactions between the various forms of phosphorus can be described by a first order equation. The concentrations of the phosphorus forms are given by D_i and the rate constants for the reactions are given by I_i.

Phosphorus was modeled as a set of first order reactions primarily because no other models were available in the literature. The first order model allows a simple analysis method for phosphorus behavior in cases where sufficient data are available to calibrate the model. In addition, some past work has indicated that first order reactions are applicable to phosphorus behavior in at least some areas.

This model is considerably simpler than most proposed phosphorus cycles because it would not be possible to determine all the rate constants involved in a complicated system. Phosphorus data are usually incomplete and it is very unlikely that enough data would exist to allow a regression analysis on many constants. The equations for this model are:

$$\frac{dD_1}{dt} = - I_1 D_1 + I_2 D_2 + I_3 D_3 - G_P P A_{DP} \quad (27)$$

$$\frac{dD_2}{dt} = - I_2 D_2 + I_1 D_1 \quad (28)$$

$$\frac{dD_3}{dt} = - I_3 D_3 + D_P P A_{DP} \quad (29)$$

where

D_1 = soluble phosphorus concentration, mg/l

D_2 = sedimentary phosphorus concentration, mg/l

I_1, I_2, I_3 = rate constants: 0.1-0.7/day

P = phytoplankton concentration, mg-C/l

A_{DP} = ratio of nitrogen to carbon in phytoplankton: 0.17 mg-N/mg-C

G_P = growth rate of phytoplankton,/day

P, G_P, and D_P are formulated in the algae model

The first order model assumes that only reactions between soluble and sedimentary phosphorus occur. This model uses the equations:

$$\frac{dD_1}{dt} = - I_1 D_1 + I_2 D_2 \qquad (30)$$

$$\frac{dD_2}{dt} = - I_2 D_2 + I_1 D_1 \qquad (31)$$

where the notation is the same as above.

The second order model uses the equation:

$$\frac{dD_1}{dt} = - I_1 D_1^2 \qquad (32)$$

Photosynthesis and Respiration of Suspended Algae

The model chosen to represent the rate of photosynthesis and respiration of suspended algae is a two term harmonic function of the form:

$$(P-R)_s = A_1 \cos(\omega t + \phi) + A_2 \cos(2\omega t + \alpha) \qquad (33)$$

where

$(P-R)_s$ = net rate of photosynthesis and respiration: $\pm(0.1\text{-}2.0)$, mg/l-day

ω = period, days

$A_1 A_2, \phi, \alpha$ = constants

This formulation was selected for two reasons. First, it is relatively simple since only three constants need to be determined (A_1,A_2 and the difference $\phi-\alpha$). The experience of previous authors in using one, two, and three term periodic functions to model diurnal variations has shown that these relatively simple expressions can be successfully applied. Second, the two term expression is more desirable than the one term expression since with two terms the maximum rate of photosynthesis need not equal the maximum rate of respiration.

An option is provided in the program which allows the user to couple this equation to the phytoplankton density. This is done simply by:

$$(P-R)_s = \beta P \qquad (34)$$

Where P is the phytoplankton concentration and β is a proportionality constant.

Photosynthesis and Respiration of Attached Algae and Benthic Plants

The model chosen to represent the net rate of photosynthesis and respiration of attached algae and benthic plants is identical to that used for the suspended algae model. It is given as

$$(P-R)_a = A_1^a \cos(\omega_a t + \phi_a) + A_2^a \cos(2\omega_a t + \alpha_a) \quad (35)$$

where

$(P-R)_a$ = net rate of photosynthesis and respiration, $\simeq$ (0.01-2.00), mg/l-day

ω_a = period, days

$A_1^a, A_2^a, \phi_a, \alpha_a$ = constants

Dissolved Oxygen

Dissolved oxygen (DO) levels in a stream are influenced by a variety of interrelated factors. The more significant factors which contribute to the change in DO levels are: 1) reaeration, 2) bacterial oxidation of organic matter, 3) algal and plant photosynthesis and respiration, 4) benthic demand, and 5) temperature variations.

The rate of reaeration of well mixed pure water is proportional to the oxygen saturation deficiency. Mathematically this can be expressed as

$$\frac{dDO}{dt} = + k_2 (DO_s - DO) \quad (36)$$

where

DO = dissolved oxygen concentration, mg/l

DO_s = saturated dissolved oxygen concentration, mg/l

k_2 = reaeration coefficient: 0.05-16.0/day

The value of DO_s for natural, unpolluted streams can be calculated from the following equation:

$$DO_s = 14.652 - 0.41022T + 0.0079910T^2 - 0.000077774T^3 \quad (37)$$

where

T = temperature, °C

Four separate models for estimating the reaeration coefficient have been included in the program. These models cover most of the work done on reaeration coefficients.

The first model for the reaeration coefficient is a general velocity-depth model of the form

$$k_2 = r_1 \frac{v^{r_2}}{h^{r_3}} \tag{38}$$

where

k_2 = reaeration coefficient,/day

v = velocity

h = depth

r_1, r_2, r_3 = constants: 2.0-12.0, 0.50-0.97, 1.67-1.75

The second model is one proposed by O'Connor and Dobbins:[2]

$$k_2 = 1109 \frac{D_m^{1/2} S^{1/4}}{h^{5/4}} \quad \text{for } C < 17 \tag{39}$$

$$k_2 = \frac{(D_m v)^{1/2}}{h^{3/2}} \quad \text{for } C > 17 \tag{40}$$

where

$$C = \frac{v}{(hS)^{1/2}}$$

D_m = liquid film diffusion coefficient: 0.01-0.02 ft^2/sec

S = river channel slope

The third model, proposed by Dobbins,[3] is given as:

$$k_2 = \frac{.2772\ C_A A E^{3/8} \coth\left(\frac{BE^{1/8}}{C_4^{1/2}}\right)}{C_4^{3/2} h} \tag{41}$$

where

$$C_4 = 0.9 + \frac{v}{\sqrt{gh}}$$

$$C_A = 1.0 + \left(\frac{v}{\sqrt{gh}}\right)^2$$

v = velocity

A = 9.68 + 0.054 (T-20)

B = 0.976 + 0.0137 $(30-T)^{3/2}$

E = 30 v s

g = gravitational constant

T = temperature, °C

s = riverbed slope

The fourth model was proposed by Thackston and Krenkel:[4]

$$k_2 = 0.0\upsilon 0299 \left[1 + \left(\frac{v}{\sqrt{gh}}\right)^{1/2}\right] \sqrt{\frac{Sg}{h}} \qquad (42)$$

The temperature dependence of the reaeration coefficient for models one, two and four above is described by the following relationship:

$$k_2 = k_2(20)\ \theta^{(T-20)} \qquad (43)$$

This relationship was chosen because it is based on extensive data and has proven reliable in many investigations.

The effects of wind on the reaeration coefficient have been observed; however, only minor theoretical treatments were found. Therefore, wind effects were not included in this model.

All models previously discussed provide input information either directly or indirectly to the dissolved oxygen model. The general equation describing the dissolved oxygen level is

$$\frac{dDO}{dt} = -k_1 L - \frac{L_d}{h} + k_2 (DO_s - DO) + (P-R)_s + (P-R)_a \qquad (44)$$

where

L = BOD, mg/l

DO = dissolved oxygen, mg/l

k_1 = deoxygenation rate for total BOD, day^{-1}

L_d = benthic oxygen demand rate, $g/m^2/day$

k_2 = reaeration coefficient, day^{-1}

$(DO_s - DO)$ = dissolved oxygen deficit

$(P-R)_s, (P-R)_a$ = photosynthesis and respiration rate for suspended and attached algae, respectively

Planktonic Algae Model

The model selected for plankton is described by the following relationships:

$$\frac{dP}{dt} = [G_p - d_p]\ P \tag{45}$$

where

$$G_p = F_1 T \left[\frac{2.718\ f}{k_e h} \left(e^{-\alpha_1} - e^{-\alpha_o} \right) \left(\frac{N}{K_n + N} \right) \left(\frac{D}{K_D + D} \right) \right] \tag{46}$$

$$d_p = F_2 T + F_3 T \tag{47}$$

D = phosphorus concentration

P = phytoplankton concentration, mg-C/l

G_p = phytoplankton growth rate, day^{-1}

d_p = phytoplankton death rate, day^{-1}

N = nitrate-nitrogen concentration, mg/l

F_1 = saturated growth rate of phytoplankton: 0.05-0.10 /day-°C

T = temperature, °C

f = photoperiod, 0.3-0.7, days

k_e = extinction coefficient: 0.1-3.0/meter

h = depth, meter

$\alpha_1 = (I_a/I_s) \exp(-k_e H)$

I_a = average incident radiation, ly/day

I_s = saturated radiation, ly/day

K_n = Michaelis constant for total inorganic nitrogen: 0.025, mg-N/l

K_D = Michaelis constant for total phosphorus: 0.006-0.025, mg-P/l

F_2 = endogenous respiration rate of phytoplankton: 0.005, /day-°C

F_3 = phytoplankton death rate due to other causes, $d^{-1}{}^{\circ}C^{-1}$

α_o = I_a/I_s, fraction of saturation light intensity: 0.5-1.0

A_{np},A_{dp} = phytoplankton nitrogen-carbon ratio: 0.05-0.17 mg-N/mg-C and phosphorus-carbon ratio: 0.024-0.24 mg-D/mg-C

Toxic Compounds

The behavior of toxic compounds in an aquatic environment is highly variable and depends upon the compound being modeled. Therefore, a simple nth order decay model was included to describe toxic compounds. This model accounts for any order of decay desired, including zero order, and can easily accommodate nonlinear behavior. The model is given as:

$$\frac{dT_c}{dt} = - aT_c^n \qquad (48)$$

where

T_c = concentration of toxic compound

a = rate constant

n = order of decay

This decay model can be used to represent any of the mechanisms of exchange, such as chemical transformation, sedimentation, biological uptake, and sorption.

Sulphite Waste Liquor

Sulphite waste liquor is included as an nth order decay reaction in the complete version of the model. Although some data were available for Pearl Benson Index in the Harbor, this parameter was not used due to a lack of waste source data.

Salinity

Salinity is treated as a conservative parameter and does not react. It is transported by applying mass balance equations. Salinity is included in the oxygen saturation calculations which in turn affect rates of reaeration.

SECTION IV

APPLICATION OF EXPLORE-I TO GRAYS HARBOR

The application of EXPLORE-I to the tidally influenced portion of Grays Harbor and the Chehalis River necessitated a number of programming changes. These changes are discussed below.

CONVERSION TO IBM

Both the hydrodynamic and water quality codes have been converted to run on an IBM computer. Program listings and card decks have been provided.

METRIC UNITS

All measurements specified in standards, reports and other documents have been expressed in metric units.

Due to the complexities of changing internal calculations, only the input and output of the code have been expressed in metric units. Parameters input in metric units are immediately converted to the English system for calculation. The calculated results are then converted to metric units for output. One exception to the above procedure is employed for the Manning coefficient, n. The value of n is commonly reported as a dimensionless quantity and was therefore not changed. Manning's n actually has units of $ft^{1/6}$.

SUBMODEL OPTION

A modification in the code allows the user to specify either the complete model or an abbreviated version which considers only a subset of parameters. The abbreviated model option evaluates the following constituents:

- Biochemical Oxygen Demand
- Dissolved oxygen
- Coliform bacteria
- Salinity (chloride)
- Toxic compound

Reaeration rates as influenced by water depth, velocity and oxygen deficits are included in the calculations. Rates of benthic oxygen demand are specified and used in the oxygen calculations.

SEAWARD BOUNDARY CONDITIONS

The seaward boundary conditions for the water quality model can be specified in several different ways. It is not necessary for all constituents to be treated in the same manner. The following options are available:

- Tidal exchange coefficient

  A tidal exchange coefficient can be specified for each constituent. If this option is used the concentration on the incoming tide will be calculated by the following equation:

$$C_{in} = \frac{\Sigma Q_{out} C_{out}}{\Sigma Q_{out}} T_i$$

where

C_{in} = concentration for incoming tide
C_{out} = concentration on ebb tide
Q_{out} = flow out
T_i = tidal exchange coefficient for constituent i

- Specified Concentration

  The concentration of each constituent can be specified as any constant or time varying value on the incoming tide.

TIDE FLAT CHANNELS

Because large areas of Grays Harbor are dry at lower low water, special consideration was given to channels which connect tide flat areas to deep channels. The bottom elevations of adjacent nodes are not used to compute a channel slope; instead, the user can specify the bottom slope of any tide flat channel by assigning the midpoint bottom elevation. This procedure was chosen to prevent excessively large calculated flows due to incorrect slopes and cross-sectional areas while allowing the tide flat nodes to "dry up."

CALIBRATION AND VERIFICATION IN GRAYS HARBOR

Data from the extensive harbor surveys conducted in 1970, 1971 and 1972 were used for calibration and verification of the estuary portion of the model. Because insufficient data were available for the complete water quality model, the abbreviated version was used.

HYDRODYNAMICS

The data summarized in the "System Layout and Data Report" were used as boundary conditions for the hydrodynamic simulation. These data represented low flow summer conditions in the study periods during 1970, 1971 and 1972. These study periods were originally chosen because of their similar tidal cycles, which permitted only one tide function to be used for all three years. In addition, a high flow case was simulated. The boundary conditions for the high flow case were chosen to simulate the Corps of Engineers[5] studies.

Because the channel dimensions used in this model were artificially created to produce the correct flows, velocities predicted by the model cannot be properly compared to field observations. However, tide heights at various locations and times, as well as direction of flow, whould be correctly simulated. Figures 6 and 7 compare the corrected tide table[6] predictions for stage and time at Pt. Chehalis and Aberdeen with the values produced by the model. It should be noted that tide table predictions are based on MLLW at the specified location and must be corrected for the horizontal datum used in the model. Figure 8 shows the elevation of MLLW compared to mean sea level at Pt. Chehalis, Aberdeen and Montesano.

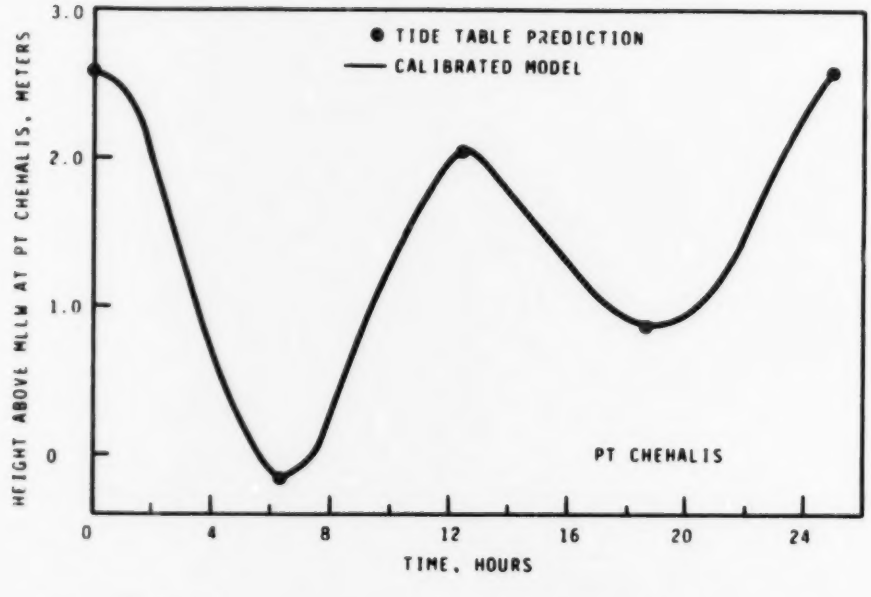


FIGURE 6. Comparison of Tide Table Predictions and Model Values

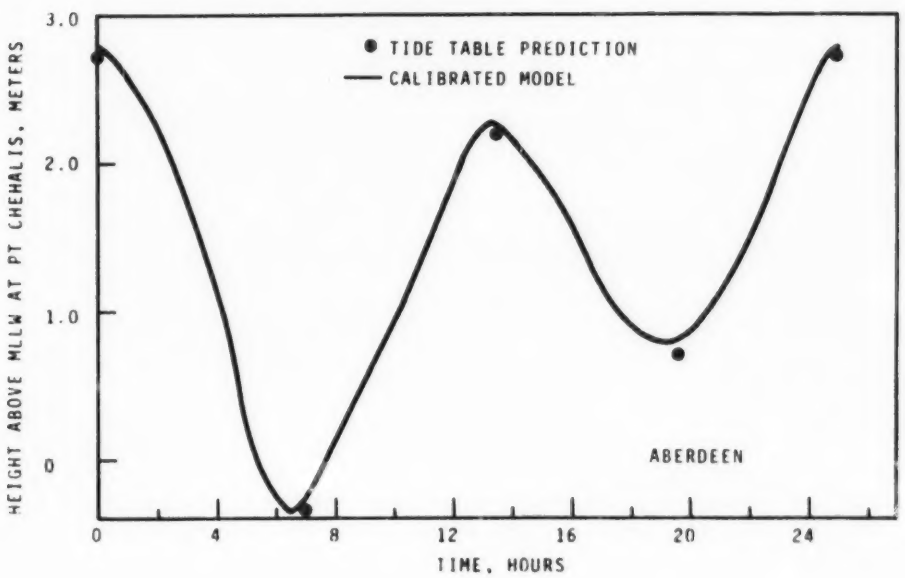


FIGURE 7. Comparison of Tide Table Predictions and Model Values

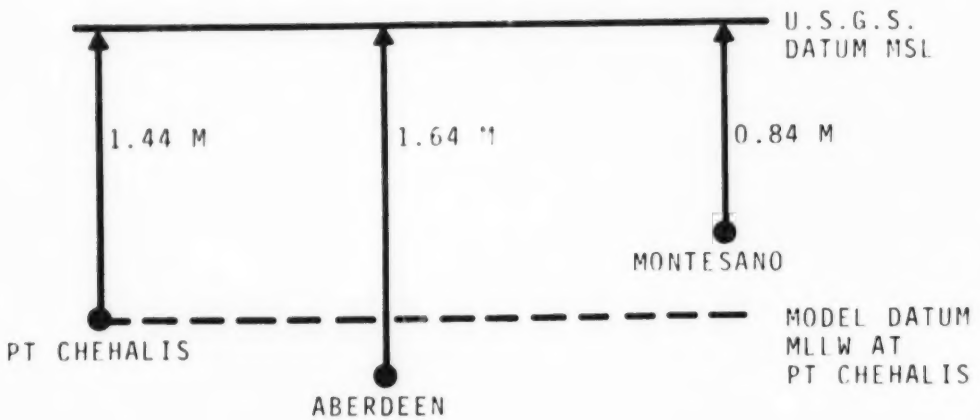


FIGURE 8. Elevation of MLLW Compared to Mean Sea Level at Pt. Chehalis, Aberdeen, and Montesano

WATER QUALITY

Figures 9, 10 and 11 show the predicted and observed oxygen concentrations in Grays Harbor. These observations were made during the Cooperative Grays Harbor Surveillance Program. The numbers on the abscissa refer to the sampling locations chosen by the State Department of Ecology. During the surveys (which took place during the periods August 10-14, 1970, August 16-20, 1971, and August 3-7, 1972), two samples were taken at each location, one 5 feet above the bottom and one 5 feet below the water surface. These two observations have been averaged for use here, so that a single point is plotted for each day. In some cases a particular station was not sampled on every day of the survey, and for this reason, or because the observations for several days were nearly identical, it was not possible to show five observations for every site. Figure 12 shows the nodalization scheme and locations of monitoring stations. Table 2 summarizes the oxygen and BOD loadings to the system for each year. Table 3 summarizes the seaward boundary conditions for each year. The constituent concentrations were held constant at these values during the incoming tide.

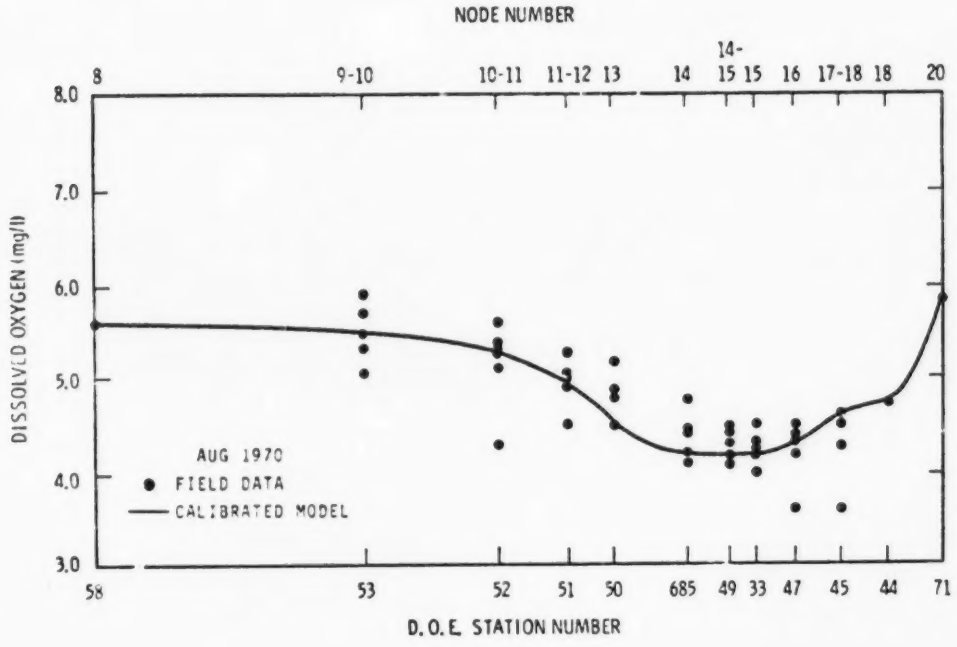


FIGURE 9. Predicted and Observed Oxygen Concentrations in Grays Harbor, August 1970

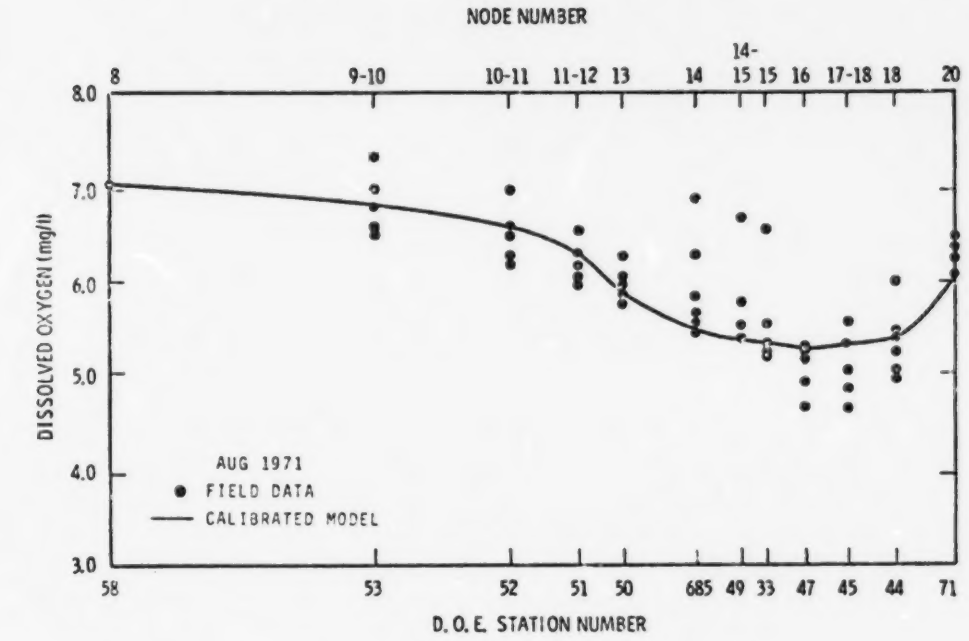


FIGURE 10. Predicted and Observed Oxygen Concentrations in Grays Harbor, August 1971

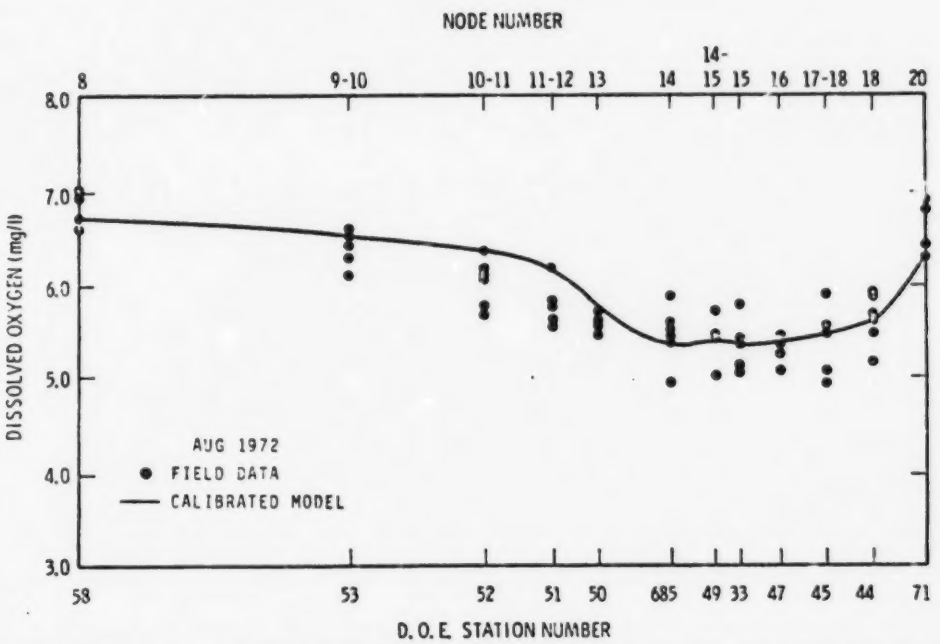


FIGURE 11. Predicted and Observed Oxygen Concentrations in Grays Harbor, August 1972

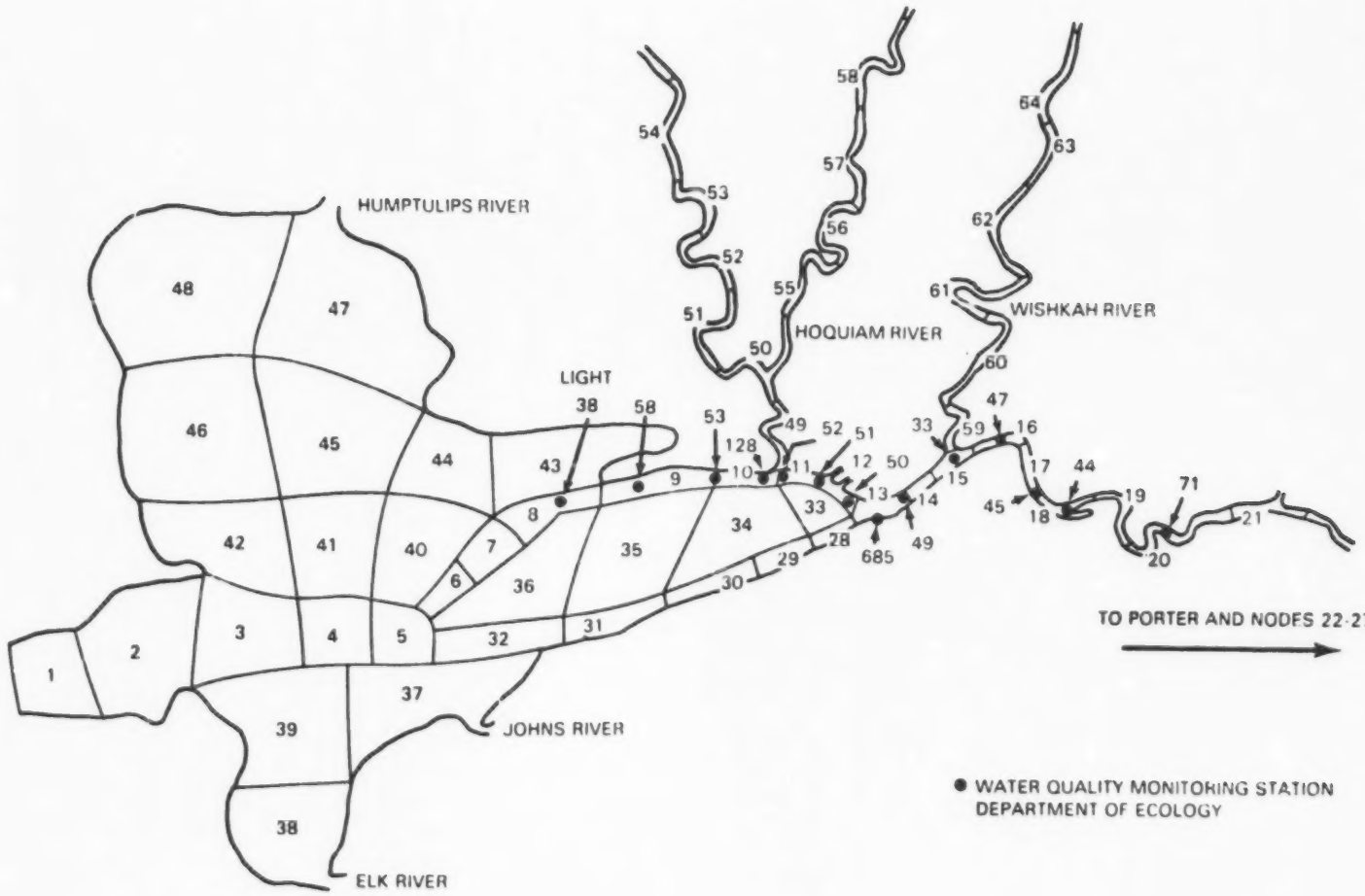


FIGURE 12. Nodalization Scheme and Locations of Sampling Stations

TABLE 2. Summary of Oxygen and BOD Inputs to Grays Harbor

Source	Node	1970 O_2 (kg/day)	1970 O_2 (mg/l)	1970 BOD (kg/day)	1970 BOD (mg/l)	1971 O_2 (kg/day)	1971 O_2 (mg/l)	1971 BOD (kg/day)	1971 BOD (mg/l)	1972 O_2 (kg/day)	1972 O_2 (mg/l)	1972 BOD (kg/day)	1972 BOD (mg/l)
Chehalis River (Porter)	27	4870	9.00	540	1.00	7620	9.00	850	1.00	8570	9.00	950	1.00
Satsop River	26	4040	9.02	450	1.00	6310	8.99	700	1.00	7100	8.99	790	1.00
Wynoochee River	23	1990	9.02	220	1.00	3100	8.99	340	1.00	3490	8.97	390	1.00
Wishkah River	15	2110	8.98	230	1.00	3300	8.99	370	1.00	3710	8.98	410	1.00
Hoquiam River	10	2110	8.80	230	0.98	3300	8.99	370	1.00	3710	8.98	410	1.00
Johns River	37	350	8.98	40	1.00	550	8.98	60	0.99	620	9.03	70	1.00
Humptulips River	47	2820	8.98	310	1.00	4400	8.99	490	1.00	4950	8.99	550	1.00
Elk River	38	350	8.98	40	1.00	550	8.98	60	0.99	620	9.03	70	1.00
ITT Rayonier	11	0	0	24940	226.48	0	0	31750	254.33	0	0	19500	227.65
Weyerhaeuser - 1	28	0	0	3040	248.30	0	0	0	0	0	0	10430	213.1
Weyerhaeuser - 2	18	0	0	450	0	0	0	1810	0	0	0	450	0
Aberdeen STP	14	50	1.68	2540	94.64	50	1.68	2540	94.33	45	1.68	2540	94.33

TABLE 3. Summary of Seaward Boundary Conditions

	Concentration in Incoming Seawater		
	Year		
Constituent	1970	1971	1972
Salinity, mg/l	15,000	15,000	15,000
BOD, mg/l	0.3	0.3	0.3
Dissolved Oxygen, mg/l	5.5	7.2	6.7

The oxygen dynamics of Grays Harbor are fairly well simulated by the model calculations. However, the effects of changes in discharge policies should be predicted with caution. There are limitations to this, and to any simulation model, which sould be pointed out.

Although the model, which was calibrated with 1970 data, made reasonably good predictions of 1971 and 1972 conditions, it is possible that other combinations of parameters could have produced similar results. It was found that the seaward boundary conditions affected dissolved oxygen concentrations significantly. The effect on the minimum oxygen concentration, however, was negligible. Figure 13 shows the results of changing the seawater DO from 6.7 to 6.0 mg/l for 1972 conditions.

The benthic oxygen demand was also found to be an important factor in regulating the oxygen concentration in the North Channel and lower Chehalis River. A uniform value of 2.0 g/m^2/day was used in nodes 9 through 18, 47 and 59 for 1970, 1971 and 1972.

Figure 14 shows calculated oxygen concentrations with and without this benthic demand for 1972 waste loads. The minimum oxygen concentration is approximately 1 mg/l greater when no benthic demand is included. The effects of reduced waste discharges on future benthic oxygen demand rates are not known.

Salinity is an important factor in Grays Harbor water quality due to its effect on oxygen saturation. For the model simulations the salinity of the incoming seawater was set at the observed value and the model allowed to run. Field observations and computed results are shown in Figure 15.

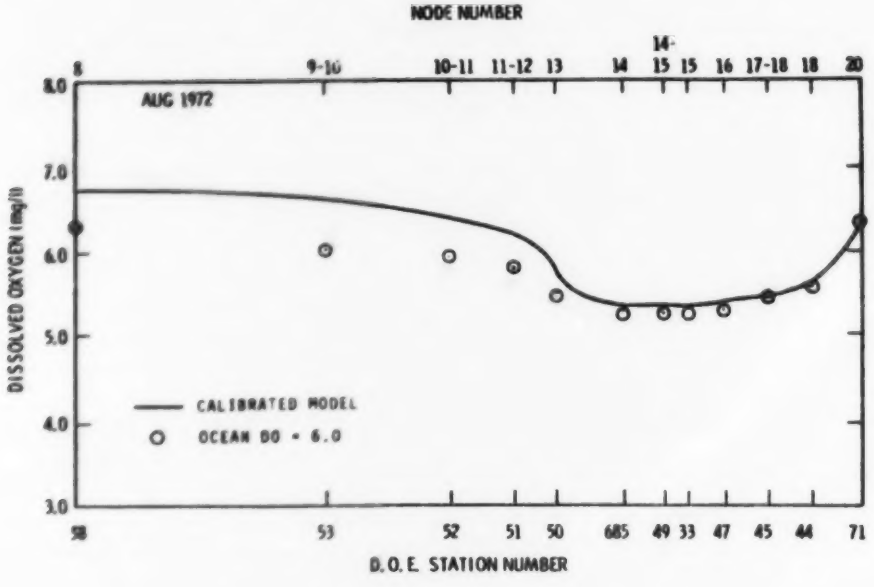


FIGURE 13. Effect of Changing Ocean Oxygen Concentration

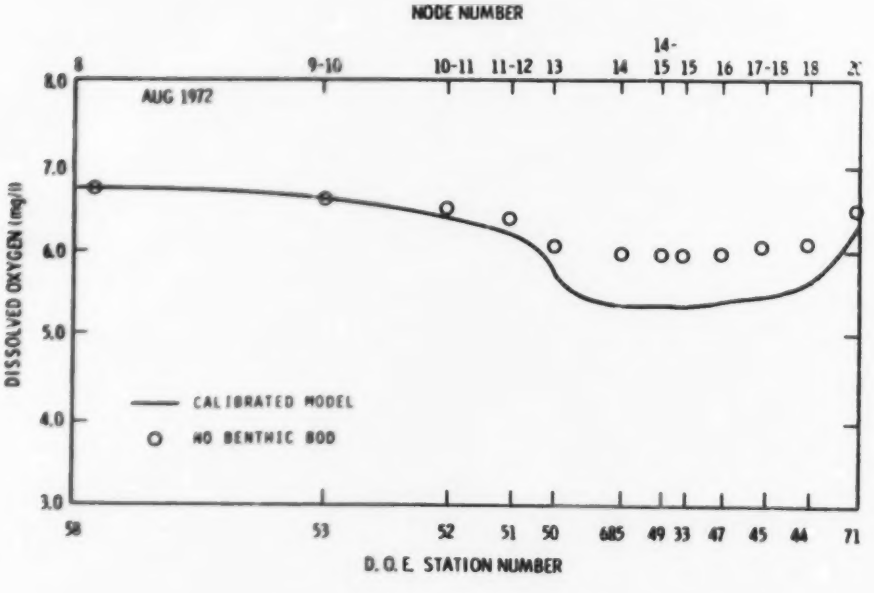


FIGURE 14. Effect of Benthic BOD on Oxygen Concentration

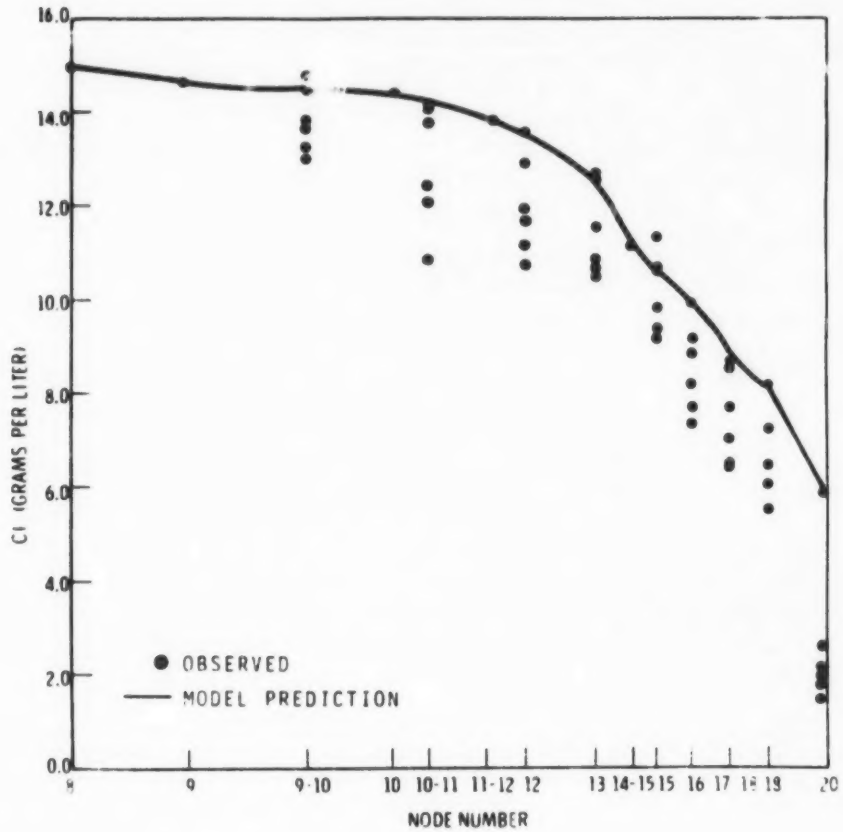


FIGURE 15. Salinity in Grays Harbor

SECTION V

DESCRIPTION OF THE PIONEER-I CODE AS APPLIED TO THE CHEHALIS RIVER

PIONEER-I is an expanded version of the DOSAG-I code which was originally developed by the Federal Water Pollution Control Administration and later revised by the Texas Water Development Board. PIONEER-I is computationally similar to DOSAG-I, but has been expanded to predict the following water quality parameters:

- Total nitrogen (conservative)
- Total dissolved solids (conservative)
- Phosphorus (first or second order reaction)
- Coliform bacteria (first order reaction)
- Ammonia (first or second order reaction)
- Nitrite (first or second order reaction)
- Nitrate (first or second order reaction)
- Biochemical oxygen demand (first order reaction)
- Chlorophyll a (coupled with the nutrients in the phosphorus and nitrogen cycles)
- Dissolved oxygen (including benthic demand, BOD, ammonia and nitrite oxidation, and algal photosynthesis and respiration as a function of chlorophyll a concentration)
- Toxic compound

The problem is solved by Lagrangian coordinates for a given set of flow conditions, waste source strengths, temperatures, and quality model reaction constants. The river system was divided into 60 reaches and a reaeration model chosen for each reach. In addition, regression constants, based on exponential fits of velocity versus flow and depth versus flow, were input for each reach. Flows were specified at headwater locations. Mean monthly temperature factors can be chosen to simulate other months of the year. The program option which permits the use of flow augmentation to maintain specified minimum DO levels in the river system is carried out by an internal iterative process. Two other options are available which allow a series of cases to be run with one input deck. Up to four BOD treatment factors can be specified and the code will perform the calculations for each factor. The other option allows up to twelve different temperatures and corresponding headwater flows to be specified; the program performs the computations for each set of values.

SOLUTION TECHNIQUE

The water quality reaction equations in the PIONEER-I water quality routing model are solved by a Lagrangian solution technique which employs a coordinate system that moves with a particle of water down the stream. The Lagrangian coordinate system allows a relatively simple computational technique to be used and reduces the computer time required to solve a given problem. It also eliminates the numerical dispersion characteristic of Eulerian solutions of the transport equation in large river systems.

Although the Lagrangian approach does not imply steady-state conditions, the manner in which it is incorporated into the model allows only the investigation of steady-state conditions. For example, the one-dimensional transport equation for BOD is:

$$V_x \frac{\partial L}{\partial x} + \frac{\partial L}{\partial t} + K_1 L = o \qquad (49)$$

where

V_x = velocity in the reach

L = BOD concentration

K_1 = BOD exertion rate constant

The method used in selecting river reaches is such that waste inputs occur at junctions between each reach and K_1 is a constant for the reach. The velocities and waste inputs are also considered constant with respect to time. The travel time through the reach is calculated from the channel velocity.

For a steady-state solution Equation 49 reduces to

$$V_x \frac{\partial L}{\partial x} = - K_1 L \qquad (50)$$

which for steady-state conditions and upon integration gives

$$L = L_o \, e^{- \frac{K_1}{V_x} X} \qquad (51)$$

WATER QUALITY MODELS

The reaction equations for each of the water quality constituents considered in PIONEER-I are discussed below.

Conservative Parameters

The modeling of conservative substances in steady-state systems is relatively simple because all reaction terms are dropped from the transport equations. Since a Lagrangian solution technique is used in PIONEER-I, only the increase or decrease in concentration due to hydraulic and quality sources must be considered. The water quality parameter concentrations are determined by a simple mass balance for each reach by the following equation:

$$C_n^i = \frac{C_{n-1}^i \, Q_{n-1} + \sum_k C_k^i \, Q_k}{Q_{n-1} + \sum_k Q_k} \qquad (52)$$

where

C_n^i = concentration of the i^{th} parameter in the n^{th} reach

C_{n-1}^i = concentration of the i^{th} parameter in the n-1 reach (the reach upstream of the n^{th} reach)

C_k^i = concentration of the i^{th} parameter in the k^{th} source or tributary at the junction of the n-1 and n^{th} reach

Q_{n-1} = flow rate in the n-1 reach

Q_K = flow rate of the k^{th} source or tributary at the conjunction of the n-1 and n^{th} reach

This method is used to determine the concentration of total dissolved solids and total nitrogen.

Phosphorus

Both first-order and second-order reactions are available in the model. If algae are present in the river system and sufficient data are available, the model shown in Figure 5 can be used. This model is described by the following first-order equations:

$$\frac{dD_1}{dt} = - J_1 D_1 + J_2 D_2$$

$$\frac{dD_2}{dt} = - J_2 D_2 + J_1 D_1 + J_3 D_3 - A_1 \qquad (53)$$

$$\frac{dD_3}{dt} = - J_3 D_3 + A_2$$

where

D_1 = areal concentration of phosphorus in sediments

D_2 = concentration of phosphorus in soluble form

D_3 = concentration of phosphorus in form of dead algae

J_1, J_2, J_3 = empirically determined rate constants

A_1 = rate of algal utilization of phosphorus, calculated by algae model

A_2 = rate of algal death calculated by algae model

Most of the phosphorus returned to the water from dead algal cells is released gradually as the algae decay. D_3 is used in the model to obtain the proper time delay in the release of the algal phosphorus.

In cases where algae are not significant or sufficient data on the algal mechanics are not available, the behavior of phosphorus can be described by a first-order reaction (see Figure 5b). Equation 53 will then reduce to

$$\frac{dD_1}{dt} = - J_1 D_1 + J_2 D_2 \qquad (54)$$

$$\frac{dD_2}{dt} = - J_2 D_2 + J_1 D_1$$

A simple second-order model is incorporated into the system (Figure 5c) for use when data are not available for evaluating the constants in the model described above or when the data indicate that a second-order reaction is occurring. The model is described by the following equation:

$$\frac{dD}{dt} = - J D^2 \qquad (55)$$

where

D = concentration of soluble and suspended phosphorus

J = decay constant

The PIONEER-I code includes all three of the above options and the appropriate mode is selected by the user.

The temperature dependence of the phosphorus rate constants J_1, J_2 and J_3 is given by the equation:

$$J_i(T) = J_k(20)\ \theta^{(T-20)} \qquad (56)$$

where

$J_i(T)$ = the value of the i^{th} constant at temperature T

$J_i(20)$ = the value of the i^{th} constant at 20°C

θ = temperature constant

T = temperature at 20°C

Coliform Bacteria

Coliform bacteria are modeled by a first-order decay equation of the form:

$$\frac{dC}{dt} = - k_c\ C_o \qquad (57)$$

where

C = coliform concentration at time t

C_o = initial coliform concentration

k_c = decay constant

The temperature dependence of the rate constant is given by:

$$k_c\ (T) = k_c\ (20)\ \theta^{(T-20)} \qquad (58)$$

where

$k_c(T)$ = decay constant at temperature T °C

$k_c(20)$ = decay constant at 20°C

θ = temperature constant

T = temperature in °C

Nitrogen

Two different models of nitrogen have been included in the PIONEER-I code. When sufficient algae data are available, the model shown in Figure 16a can be used. This model can be described by the following first order equations:

$$\frac{dC_1}{dt} = - I_1C_1 + I_3C_4 \qquad (59)$$

$$\frac{dC_2}{dt} = - I_2C_2 + I_1C_1$$

$$\frac{dC_3}{dt} = + I_2C_2 - B_1$$

$$\frac{dC_4}{dt} = - I_3C_4 + B_2$$

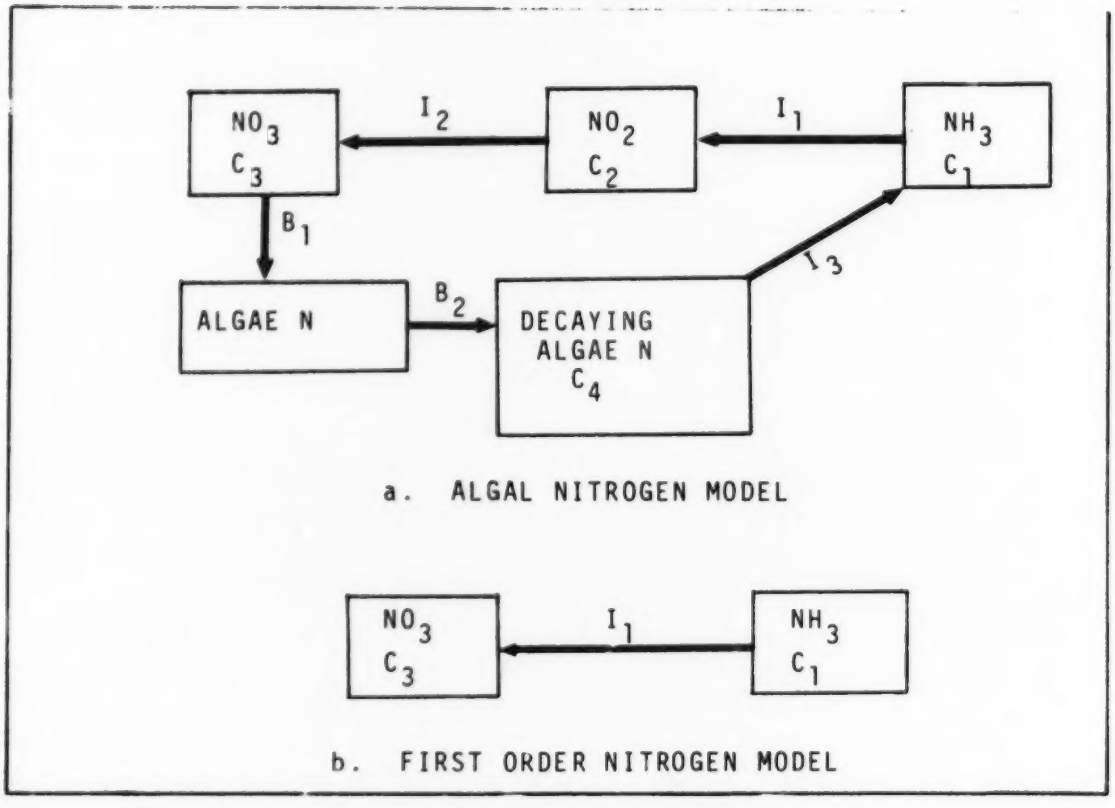


FIGURE 16. Nitrogen Models

where

C_1 = concentration of ammonia nitrogen

C_2 = concentration of nitrite nitrogen

C_3 = concentration of nitrate nitrogen

C_4 = concentration of nitrogen in decaying algae

I_1, I_2, I_3 = empirically determined rate constants

B_1 = rate of algal utilization of nitrogen calculated by the algae model

B_2 = rate of algal death calculated by the algae model

The nitrogen in decaying algae is accounted for separately to obtain the proper time delay in nitrogen release from decaying algae.

In many cases algae are not present or a lack of data precludes the use of algal interaction with nitrogen, so a simple oxidation scheme (as shown in Figure 16b) can be used. The equations for this model are

$$\frac{dC_1}{dt} = - I_1 C_1$$

$$\frac{dC_3}{dt} = + I_1 C_1 \qquad (60)$$

The dissolved oxygen used in the ammonia and nitrite oxidation processes is determined stoichiometrically from the following equations.

$$NH_4^+ + \frac{3}{2} O_2 \rightarrow NO_2^- + 2H^+ + H_2O$$

$$NO_2^- + \frac{1}{2} O_2 \rightarrow NO_3^- \qquad (61)$$

The dissolved oxygen consumed by oxidation of ammonia and nitrite is transferred from the dissolved oxygen model.

The effect of temperature on the nitrogenous oxidation process is accounted for by the expression:

$$J_i(T) = J_i \ (20) \ \theta^{T-20} \qquad (62)$$

where

$J_i(T)$ = i^{th} rate constant of temperature T

$J_i(20)$ = i^{th} rate constant at 20°C

θ = empirically derived constant

T = temperature °C

Biochemical Oxygen Demand (BOD)

The suspended and dissolved BOD is described by the equation:

$$\frac{dL}{dt} = - (k_1 + k_3) L + P \qquad (63)$$

where

L = BOD concentration

k_1 = deoxygenation rate constant

k_3 = sedimentation rate constant for suspended BOD

P = scour of BOD from the river bottom

The temperature dependence of the deoxygenation coefficient k_1 is given by:

$$k_1(T) = k_1(20)\ \theta^{(T-20)} \qquad (64)$$

where

$k_1(T)$ = k_1 at temperature T °C

$k_1(20)$ = k_1 at 20°C

θ = constant

Algae Model

The modeling of algae is inherently complex because of the heterogeneous algal populations and the myriad of interacting environmental factors that influence algal dynamics.

Most phytoplankton models are based on calculation of the growth and death rates of the algae, coupled with a system of equations describing the predator and prey relationships. These models, however, predict long-term (weeks or months) dynamics of the phytoplankton concentration. Steady-state models applicable to the modeling effort proposed here have not, in general, been attempted.

The algae model in the PIONEER-I code considers the growth and death of phytoplankton on the basis of the following equation:

$$\frac{dP}{dt} = (G - d)\ P \qquad (65)$$

where

P = phytoplankton concentration

G = phytoplankton growth rate

d = phytoplankton death rate

Numerous forms of growth and death terms have been used in previous models. One of the most complete forms is given by DiToro, et al.;[7]

$$G = [F_1 T] \times \left[\frac{2.718f}{k_e H}\left(e^{-\alpha_1} - e^{-\alpha_o}\right)\right]\left[\frac{N}{K_N+N} \cdot \frac{D}{K_D+D}\right]$$

$$d = F_2 T + F_3$$

where

F_1 = saturated growth rate of phytoplankton

F_2 = respiration rate of phytoplankton

F_3 = death of phytoplankton due to other causes

T = temperature

f = average photoperiod

k_e = extinction coefficient

H = average water depth

$\alpha_1 = (I_a/I_s) \exp\{-k_e H\}$

$\alpha_o = I_a/I_s$

I_a = average irradiance incident on water surface

I_s = irradiance at which saturated growth occurs

N = nitrogen concentration

K_N = Michaelis constant for nitrogen

D = phosphorus concentration

K_D = Michaelis constant for phosphorus

The growth rate considers three effects: the first factor represents the normal saturated growth of the phytoplankton as a function of temperature; the second factor considers the reduction in growth due to the average irradiance available to the phytoplankton for photosynthesis; and the third factor accounts for the decrease in growth rate due to nutrient deficiency (phosphorus and nitrogen).

Dissolved Oxygen (DO)

The dissolved oxygen concentrations in a stream are influenced by a variety of interrelated factors, of which the most important are

- bacterial oxidation of organic matter
- benthic demand
- algal photosynthesis and respiration
- reaeration
- temperature

The first four categories represent more or less independent phenomena, all of which are influenced by temperature. The equation for the dissolved oxygen represents a mass balance of these sinks and sources:

$$\frac{dDO}{dt} = - \text{(BOD use)} - \text{(Benthic use)} \pm \text{(Algal production or use)} + \text{(Reaeration)} \qquad (66)$$

The rate of oxygen use in the degradation of carbonaceous BOD is given by the expression:

$$BOD_C = k_1 L \text{ mg/l/day} \qquad (67)$$

The carbonaceous BOD concentration (L) as a function of river reach is computed by the BOD model.

For nitrogenous oxidation, the stoichiometric coefficients are used to convert to oxygen use:

$$BOD_N = I_1 C_1 N_1 + I_2 C_2 N_2 \text{ mg/l/day} \qquad (68)$$

where

C_1 = concentration of ammonia nitrogen

C_2 = concentration of nitrite nitrogen

I_1, I_2 = rate constants

N_1, N_2 = stoichiometric coefficients relating oxygen to ammonia nitrogen and nitrite nitrogen, respectively

The ammonia and nitrite concentrations are computed as a function of river reach by the nitrogen model.

In any steady-state model, the benthic oxygen demand must be input in the form of an areal demand, B_e, $g/m^2/day$. The benthic demand is computed by the following relationship:

$$\text{Benthic} = \frac{B_e}{H} \text{ mg/l/day} \tag{69}$$

where H is the river depth. The benthic demand is input for each river reach.

The oxygen produced by photosynthesis can be calculated in one of two ways. First, if algae calculations are being used by the model, the net DO production will be given by:

$$(P\text{-}R)_{Net} = a\ P \tag{70}$$

where

$(P\text{-}R)_{Net}$ = net DO production
a = proportionality constant
P = phytoplankton concentration

The phytoplankton (chlorophyll a) concentration is calculated by the algae model. If no algae calculations are being performed, the net DO production can be input as a constant for each reach of the river.

The prediction of reaeration rates (k_2) is a very important part of any DO balance in a river system The PIONEER-I model provides a choice of four reaeration models for each reach:

- specific k_2 value
- velocity and depth exponent model
- flow exponent model
- Thackston-Krenkel slope dependent model

A specific value of k_2 may be read into the program if, for example, field surveys have been made at particular flows and values of the reaeration coefficient have been computed from the results. This option must be used with caution since the reaeration coefficient is generally a function of stream properties such as water velocity and depth.

The second option is based on observation that the reaeration rate coefficient is directly proportional to the mean stream velocity and inversely proportional to the mean depth. This relationship assumes that increasing velocity and turbulence increases the surface renewal rate of dissolved oxygen and promotes mixing and dispersion of the oxygen throughout the depth of the stream. In addition, increased depth decreases the rate of dispersion of dissolved oxygen throughout the water mass, resulting in lower quantities of oxygen being transferred from the atmosphere.

For this option:

$$k_2 = a\frac{v^b}{h^c} \qquad (71)$$

where

v = velocity (m/sec)

h = depth (m)

a,b,c = regression coefficients

Numerous investigators have determined the coefficients for use in Equation 71 to calculate the reaeration coefficient for any stream in which the mean velocity and mean depth are known. Table 4 presents these coefficients as determined by five investigators in both field and laboratory tests. The coefficients developed by Churchill in 1962 and by Langbein and Durum in 1967 are probably the best known for the computation of the reaeration rate coefficient for general model use.

TABLE 4. Coefficients for Computation of the Reaeration Coefficient (converted to metric units)

Investigator	Reference	a	b	c
Churchill, et al.	8	2.178	0.969	1.673
Langbein and Durum	9	1.23	0.50	1.33
O'Connor and Dobbins	2	3.93	0.50	1.50
Owens and Gibbs	10	2.31	0.67	1.85

The third option for computing the reaeration coefficient is given by

$$k_2 = aQ^b \tag{72}$$

where

Q = flow

a,b = regression coefficients

At the present time no generally acceptable values for a and b are available because many of the factors which affect reaeration are not adequately described by a simple relationship with stream flow.

The fourth option is based on a formulation by Thackston and Krenkel.[4]

$$k_2 = 0.0\,0\,.\,5 \left(1 + \left(\frac{v}{(gd)^{1/2}}\right)^{1/2}\right) \cdot (S)^{1/2} \left(\frac{g}{a}\right) \tag{73}$$

where

v = velocity

g = gravity constant

d = depth

S = slope

The slope is input by the user. This formulation is based primarily on laboratory data.

The reaeration coefficient calculated by the above equations is corrected for temperature on the basis of the following equation:

$$k_2\ (T) = k_2\ (20)\ (1.0159)^{(T-20)} \tag{74}$$

where

k_2 (T) = reaeration coefficient at temperature T °C

k_2 (20) = reaeration coefficient at 20°C

T = temperature, °C

The contribution of dissolved oxygen from reaeration is calculated by:

$$\text{Reaeration} = k_2\ (DO_{Sat} - DO) \tag{75}$$

where

DO_{Sat} = saturated DO concentration at the temperature, salinity, and elevation of the reach

k_2 = reaeration calculated by one of the four models given above

The actual DO equation is then written as:

$$\frac{dDO}{dt} = - k_1 L - (I_1 C_1 N_1 + I_2 C_2 N_2) - \frac{B_e}{H} + a P + k_2 (DO_{Sat} - DO) \quad (76)$$

General N^{th} Order Reaction Model

Although not specifically requested, a general N^{th} order reaction model has been incorporated in the PIONEER-I model to allow the user the flexibility of using higher order reaction kinetics. The equation describing this model is:

$$\frac{dS}{dt} = - KS^n \quad (77)$$

where

n = any real number specified by the user

S = concentration of specific compound

K = rate constant

This model can be used in place of the BOD, nitrogen and phosphorus models or can be used to study the distribution of various toxic or other compounds in the river system. Inclusion of this model adds negligible computer running time or input complication and may prove very useful at a later time in analyzing miscellaneous reactions in the stream.

Integrated Water Quality Models

The integrated water quality models are shown in Figure 17. The set of differential equations presented above are solved along each reach using a fourth order Runge-Kutta procedure. This solution technique is computationally fast, yet accurate enough for the relatively slowly varying functions used in the water equations.

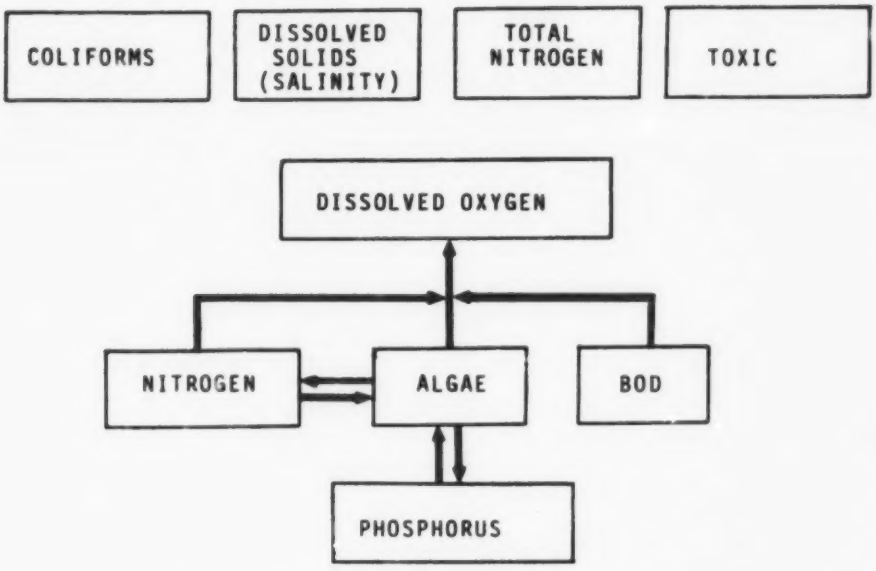


FIGURE 17. Integrated Water Quality Models

PROGRAM SETUP AND OPERATION

The river basin being modeled must be divided into a number of discrete elements for input into the PIONEER-I program. These elements are defined in the DOSAG-I code as follows:

- junction - the confluence of two streams within the river basin being simulated
- stretch - a river portion between junctions
- headwater stretch - the length of a river or stream from its headwater to its first junction with another stream
- reach - a subunit within a stretch (either a headwater stretch or a regular stretch)

Normally a reach is defined as any place in a stretch where there is a significant change in the hydraulic, biological or physical characteristics of the river, the addition of a waste load, or the withdrawal of water from the river. The

PIONEER-I code requires that the headwater stretches be numbered consecutively, beginning with one. The nonheadwater stretches can be numbered in any manner. The current PIONEER-I code has the following restrictions:

- maximum number of headwater stretches = 25
- maximum number of junctions = 25
- maximum number of reaches = 300
- maximum number of stretches = 50
- maximum of 12 months of routing for temperature and headwater flows
- maximum number of dissolved oxygen targets = 4 (a minimum of one dissolved oxygen target must be specified, which may be entered as a negative number if no flow augmentation is desired)
- maximum of five degrees of treatment for waste influents
- maximum of 40 reaches per stretch

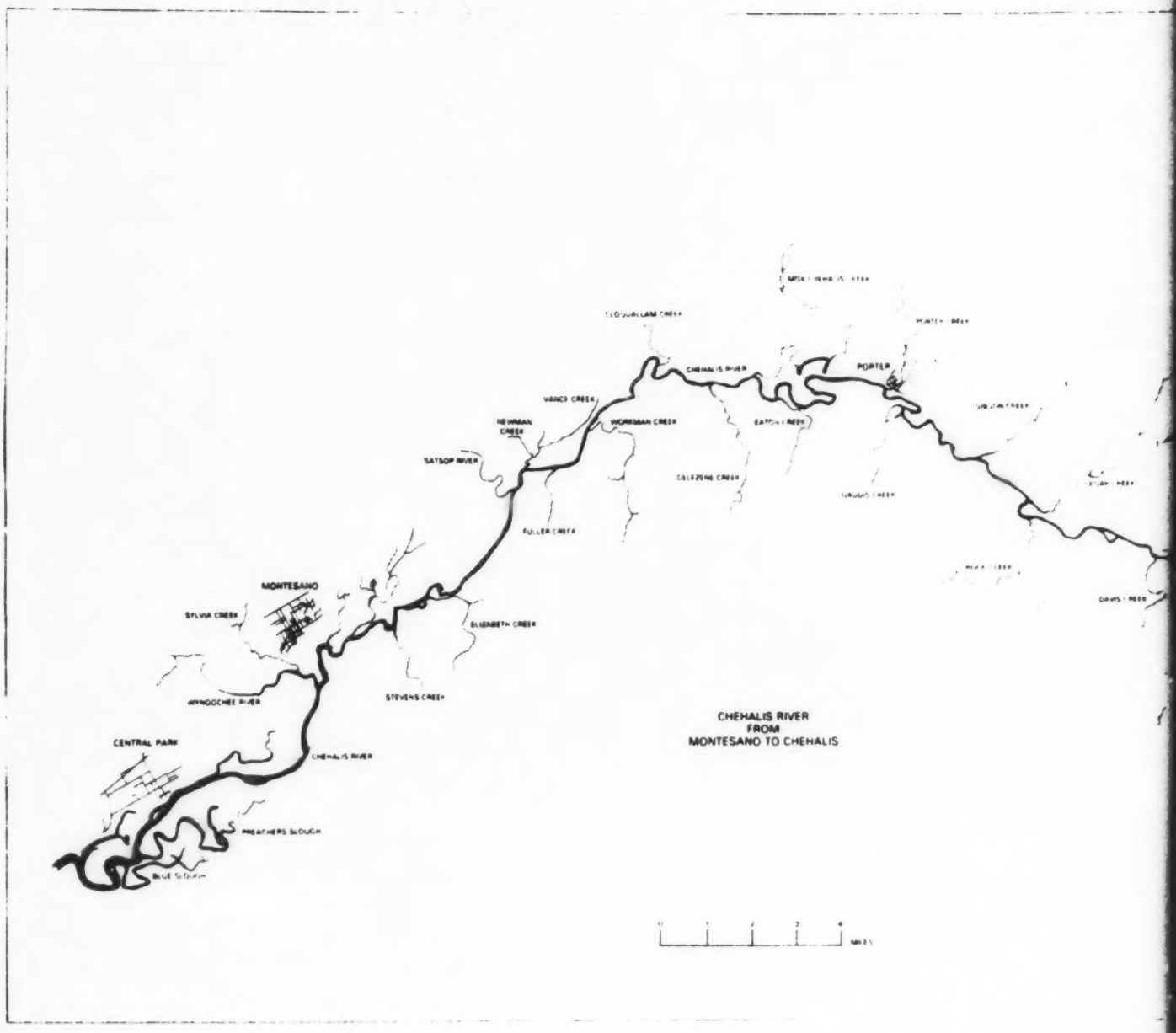
The methods of input for the hydraulic and physical characteristics and the models of reaeration for the reaches in the stream system being simulated are essentially the same as they were for DOSAG-I and are not discussed here. The handling of waste discharges and diversions is also identical to DOSAG-I.

With DOSAG-I, temperatures for all reaches in the simulation were the same and this temperature value was input via the file H card (file H - mean monthly temperatures). The use of a uniform temperature over the entire river basin is not always a valid assumption, however, and PIONEER-I requires that temperature be input for each reach on the file F-3 cards. In order to facilitate the multiple run capability available with DOSAG-I the file H cards in PIONEER-I now specify a mean monthly temperature factor. The temperature for each reach is then calculated in PIONEER-I by multiplying the reach temperature input on the file F-3 card by the mean monthly temperature factor specified for the current run on the file H card.

PIONEER-I offers a choice of quality models to be used in the simulation. File J has been added to allow the PIONEER-I user to select the desired quality models. The options available and input formats are discussed in detail in the "User's Manual."

APPLICATION OF PIONEER-I TO THE CHEHALIS RIVER

The Chehalis River from Chehalis to Montesano was subdivided as described in the Data Report. Figure 18 shows the river, tributaries and those waste sources identified.


CHEHALIS RIVER
PORTER
VANCE CREEK
NEWMAN CREEK
NOREMAN CREEK
SATSOP RIVER
MONTESANO
SYLVIA CREEK
ELIZABETH CREEK
STEVENS CREEK
WYNOOCHEE RIVER
CENTRAL PARK
CHEHALIS RIVER
PREACHERS SLOUGH
CHEHALIS RIVER
FROM
MONTESANO TO CHEHALIS

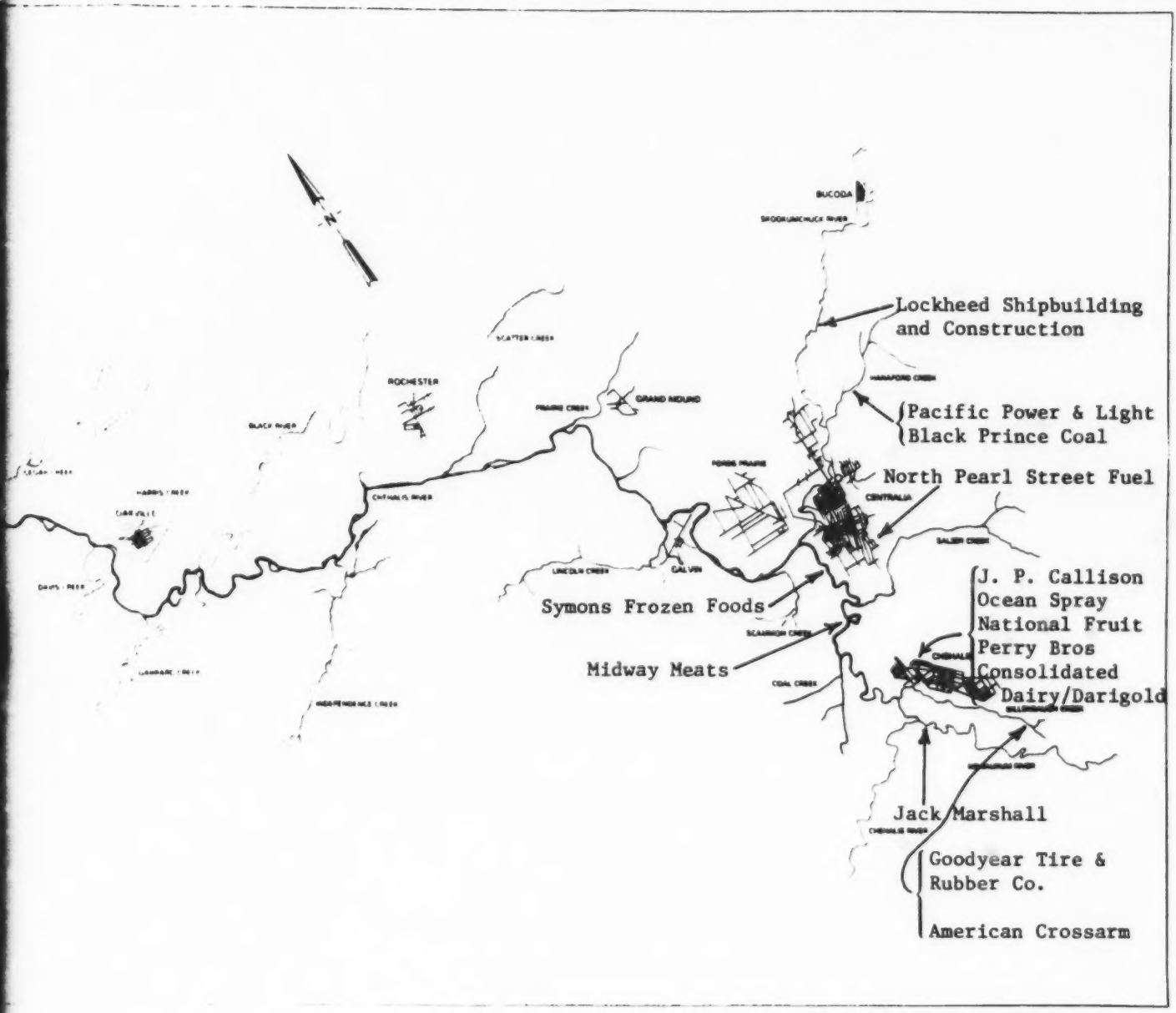


FIGURE 18. Waste Sources on the Chehalis River and Its Tributaries

Because the data collection effort was unsuccessful in obtaining water quality data for most of the waste sources, calibration and verification were not possible. However, the PIONEER-I model was set up and run with assumed values of waste source parameters. Several runs were made in order to demonstrate the proper functioning of the model.

The results of these runs are presented in Figures 19 through 22.

Figure 19 shows the two flow cases examined. The low flow corresponded to the summer conditions analyzed in the harbor area and the high flow case corresponded to the flows during the Corps of Engineers[5] study.

Because no significant waste sources were documented for the Chehalis River an arbitrary source of 13,000 Kg/day of BOD was placed at River Kilometer 96.7 to test the operation of the model. Figure 20 shows the calculated BOD and dissolved oxygen for the low flow case and the general variation model. In analyzing these results it was found that quite high reaeration coefficients were being calculated (12/day). The high values were the result of the low flow conditions and the fact that the model does not allow changing channel widths with flow. Therefore, a low flow dictates a very shallow depth and high reaeration coefficient.

Figure 21 shows the calculated DO and BOD for the same case except that the reaeration coefficient was constrained to be less than or equal to 3 $days^{-1}$. This constraint has been left in the model. Placing this upper limit on the reaeration coefficient resulted in a significant oxygen lag curve, as shown in Figure 21.

Figure 22 shows the same case as Figure 21 except that the river flow was substantially greater. The oxygen sag curve was much less pronounced for this case.

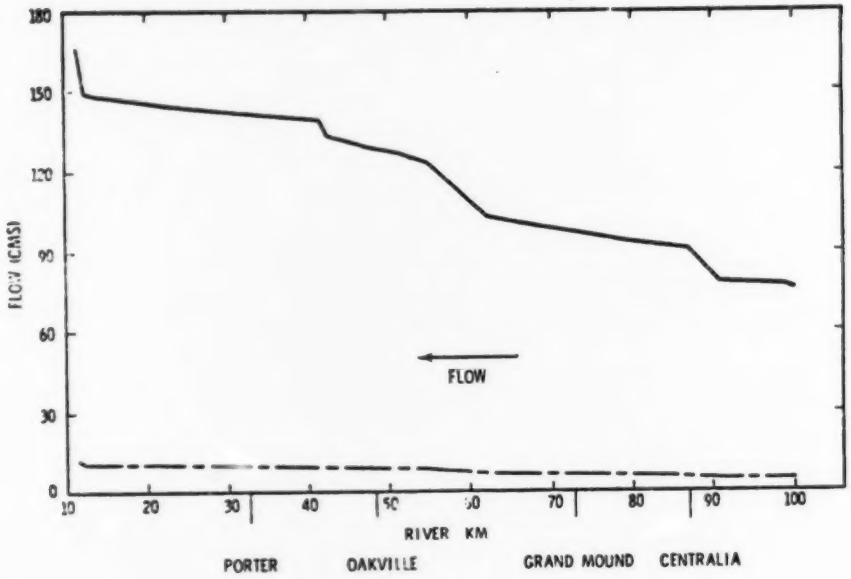


FIGURE 19. High and Low Flow Versus River Kilometer in the Chehalis River

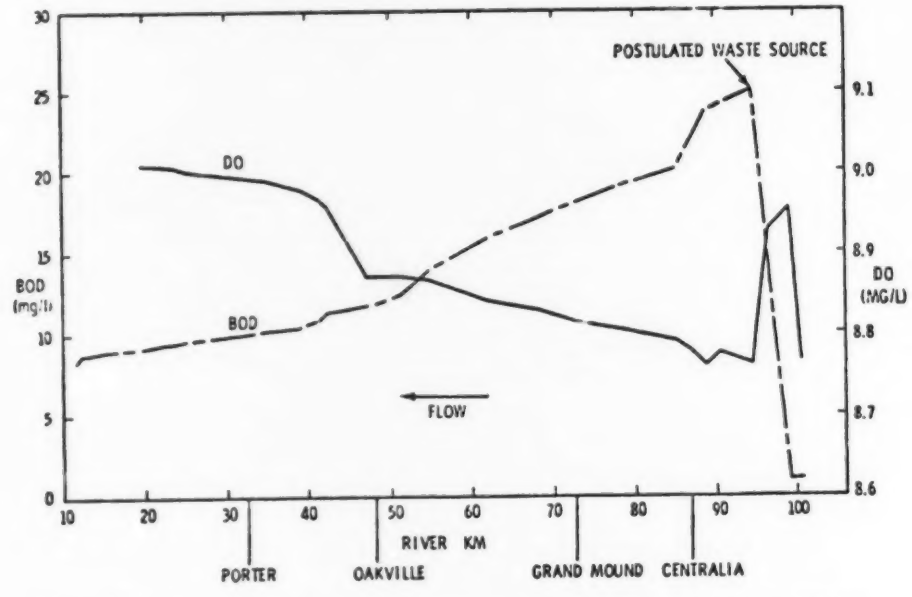


FIGURE 20. Dissolved Oxygen and BOD for Low Flow Case, General Reaeration Model

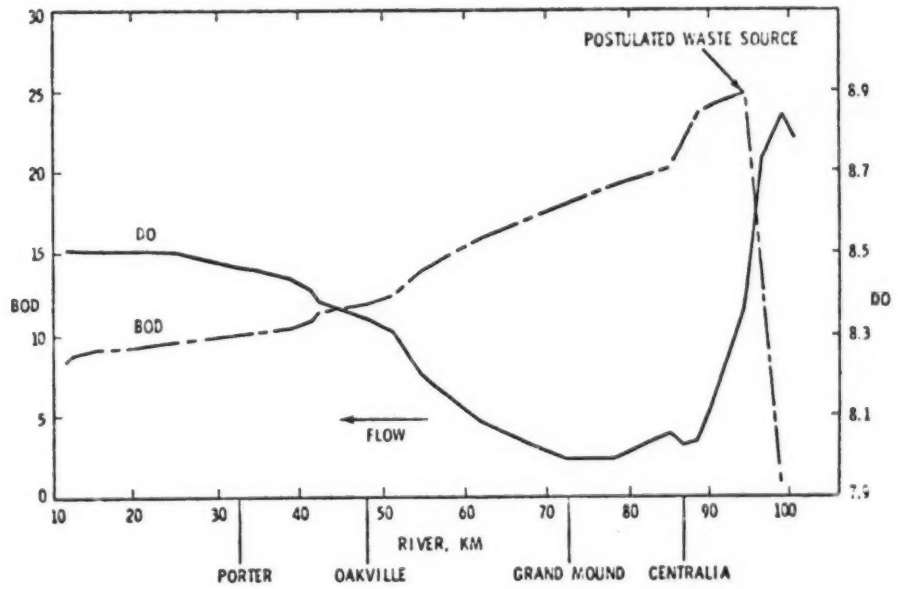


FIGURE 21. Dissolved Oxygen and BOD for Low Flow Case, Reaeration Coefficient ≤ 3 Days^{-1}

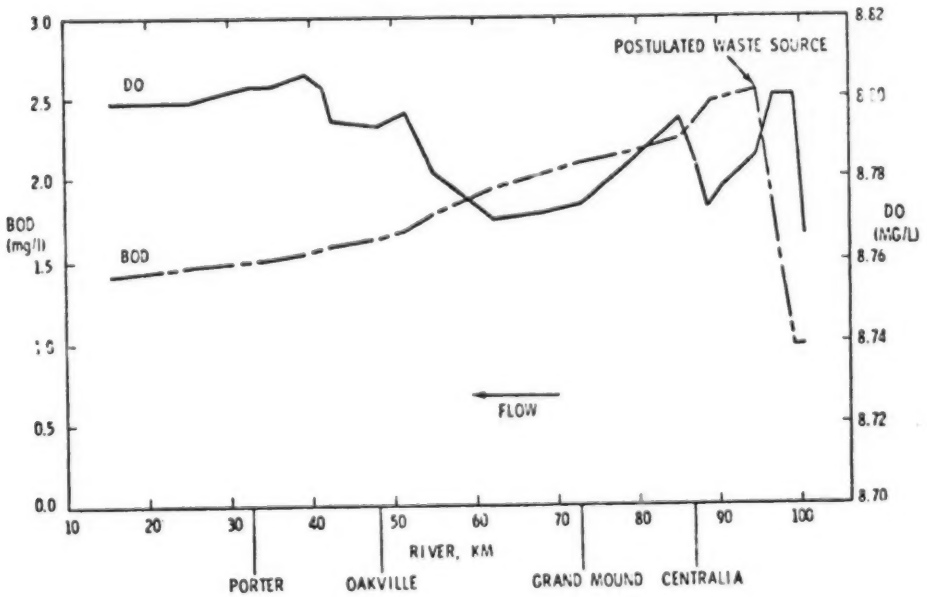


FIGURE 22. Dissolved Oxygen and BOD for High Flow Case, General Reaeration Model

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